

## Review Paper on Numerical Investigation of Multi-Fuel (Diesel + Hydrogen + Biofuel)

### Combustion in CI Engines Using CFD

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#### Abstract

This review paper examines the numerical investigation of multi-fuel combustion involving diesel, hydrogen, and biofuel in compression ignition (CI) engines using Computational Fluid Dynamics (CFD). The growing demand for cleaner and more efficient combustion technologies has spurred interest in alternative fuels and their blends. This paper discusses the methodology, key findings, and challenges associated with the CFD analysis of multi-fuel combustion, emphasizing the synergetic effects of hydrogen and biofuels on diesel combustion. The review aims to provide insights into optimizing fuel blends for improved engine performance and reduced emissions.

*Keywords:* CFD, Bio-Diesel, biofuel, CI Engine, ICE.

#### 1. Introduction

The internal combustion engine (ICE) industry is under significant pressure to reduce emissions and improve fuel efficiency due to stringent environmental regulations and the depletion of fossil fuel reserves. Multi-fuel combustion, which involves blending conventional diesel with alternative fuels such as hydrogen and biofuels, offers a promising

solution. This review paper focuses on the numerical investigation of such multi-fuel systems in CI engines using CFD.

#### 1.1 Compression Ignition (CI) Engines

Compression ignition dual fuel engines have been recognized as an attractive combustion mode for their potential to burn gaseous fuels at a thermal efficiency comparable to diesel engines and reduced PM emissions. Numerous researchers have examined the combustion process of dual fuel engines. For example, Karim [3] examined the heat release process derived from cylinder pressure and classified the heat release process of dual fuel combustion into three modes: (1) the ignition of the pilot fuel, which usually has higher reactivity than gaseous fuels fumigated into the intake mixture; (2) the concurrent combustion of diesel and NG presented within the diesel spray plume, (3) the combustion of a diesel free, NG-air mixture. The research conducted in the past decades has focused on the detailed experimental measurement of the impacts of engine speed [5,6], load [7–9], substitution ratio of NG [5,10], exhaust gas recirculation (EGR) [10,11], the mass of NG injected into intake manifold [12], and the amount of

diesel fuel injected in each cycle [13] in the dual fuel engine combustion process.

Recently, there has been increasing interest in examining the impact of pilot fuel injection timing and injection pressure on the combustion process and exhaust emissions from dual fuel engines [13–17]. The combustion process of NG was controlled by the mixing processes of the pilot fuel with the premixed charge (i.e. no flame propagation or bulk ignition) and whether or not the premixed NG-air mixture is too lean to support the propagation of the turbulent flames if initiated by pilot fuel. Past research on the combustion process of NG-diesel dual fuel engines has focused on the overall heat release process of NG and pilot diesel. In comparison, to the best of our knowledge, little research on the combustion process of gaseous fuels, such as methane, in dual fuel engines has been conducted. It is technically difficult to split the heat release of dual fuel engines to that of pilot fuel and gaseous fuel, respectively.

## 1.2 Computational Fluids Dynamics (CFD)

The computational fluids dynamics (CFD) modeling has been recognized as a platform for the investigation of the combustion process of internal combustion engines, especially compression ignition engines involving diffusion combustion. A CFD model coupled with a chemical kinetic mechanism has been applied to simulate the diesel injection process, the formation of diesel-NG-air mixture, oxidation of diesel and methane, and the formation

of pollutants including mainly nitrogen oxide ( $\text{NO}_x$ ) in NG-air dual fuel engines. For example, Liu et al. [29] simulated the combustion characteristics of a dual fuel engine with a swirl chamber using the CFD software KIVA-3 as a platform. The model coupled with fuel chemistry was able to predict the combustion process and the formation of  $\text{NO}_x$  in a light-duty 4-cylinder NG-diesel dual fuel engine. Nieman et al. [30] numerically investigated the operation of a NG-diesel dual fuel engine operated on the reactivity controlled compression ignition (RCCI) mode using a KIVA 3V CFD code and were able to simulate the formation of soot,  $\text{NO}_x$ , CO, and unburned hydrocarbon (UHC) emissions.

Maghbouli et al. [28] numerically investigated the impact of multi-pulse pilot fuel injection strategies on the combustion process of a dual fuel engine. The impact of injection timing of the 1st and 2nd injection pulse on the combustion process, exhaust emissions and the contribution of diesel to the total energy were simulated. It was evident that the previous numerical studies on dual fuel engines have focused on the overall heat release process and formation of pollutants in cylinder. In comparison, the consumption of methane in each combustion stage and mechanism for methane to survive the main combustion and the post-combustion oxidation process have never been reported by any numerical study. The knowledge needed in evaluating the extent of success of engine operation and control

strategy in minimizing methane emissions is not available.

### 1.3 Importance of Multi-Fuel Combustion

1. **Emissions Reduction:** Hydrogen and biofuels can significantly reduce harmful emissions compared to pure diesel.

2. **Renewable Energy Utilization:** Biofuels are derived from renewable resources, contributing to sustainability.

3. **Improved Combustion Efficiency:** The high reactivity of hydrogen can enhance the combustion process.

## 2. Methodology

### Computational Fluid Dynamics (CFD) in Combustion Studies

CFD is a powerful tool for simulating and analyzing the complex processes involved in combustion. It allows for detailed examination of fluid flow, heat transfer, and chemical reactions within the engine cylinder.

1. **Governing Equations:** The primary equations used in CFD include the Navier-Stokes equations for fluid flow, energy conservation equations, and species transport equations for chemical reactions.

2. **Turbulence Modeling:** Accurate modeling of turbulence is crucial for predicting the mixing and combustion processes. Common models include  $k-\epsilon$ ,  $k-\omega$ , and Large Eddy Simulation (LES).

3. **Chemical Kinetics:** Detailed chemical mechanisms for diesel, hydrogen, and biofuels are incorporated to simulate the combustion process.

## 2.1 Fuel Blends

### 2.1.1. Diesel-Hydrogen Blends:

**Properties:** Diesel is a conventional hydrocarbon fuel with a high energy density and relatively low reactivity. Hydrogen, on the other hand, has a high flame speed, low ignition energy, and high diffusivity, making it highly reactive.

**Blend Ratios:** Different volumetric or mass-based ratios of diesel and hydrogen are used to investigate their combined effects on combustion. Typical blend ratios might include 90% diesel - 10% hydrogen, 80% diesel - 20% hydrogen, etc.

### 2. Diesel-Biofuel Blends:

**Properties:** Biofuels such as biodiesel and ethanol are renewable fuels with lower carbon footprints. Biodiesel typically has higher oxygen content, which can improve combustion efficiency and reduce soot formation. Ethanol has a high octane number and can reduce knocking in engines.

**Blend Ratios:** Various ratios of diesel and biofuel are explored, such as 80% diesel - 20% biodiesel, 70% diesel - 30% ethanol, etc.

### 3. Multi-Fuel Blends (Diesel + Hydrogen + Biofuel):

**Properties:** Combining diesel, hydrogen, and biofuel aims to leverage the benefits of each fuel

type. Hydrogen's high reactivity can enhance the combustion of diesel, while the oxygen content in biofuels can lead to cleaner combustion.

**Blend Ratios:** Different combinations are studied, such as 70% diesel - 15% hydrogen - 15% biodiesel, 60% diesel - 20% hydrogen - 20% ethanol, etc.

### 3. Combustion Models

#### 3.1. Eddy Dissipation Concept (EDC):

**Description:** The EDC model is widely used for turbulent combustion modeling. It assumes that the reaction rate is controlled by the rate of turbulent mixing on the smallest scales (eddies).

**Application:** Suitable for capturing the interactions between turbulence and chemical reactions in CI engines, especially for fuels with different reactivities like diesel and hydrogen.

#### 3.2. Flamelet Generated Manifold (FGM):

**Description:** The FGM model simplifies the combustion process by precomputing flamelet libraries that represent the local flame structure. These libraries are then used during the CFD simulation.

**Application:** Useful for handling complex chemical kinetics of multi-fuel blends, as it reduces the computational cost while maintaining accuracy in capturing the combustion process.

#### 3.3. Partially Premixed Combustion (PPC)

**Model:**

**Description:** The PPC model addresses combustion regimes where the fuel and air are not fully mixed before ignition. It captures the transition from premixed to diffusion-controlled combustion.

**Application:** Relevant for multi-fuel blends where partial premixing occurs, especially when using high-reactivity fuels like hydrogen alongside diesel.

#### 3.4. Chemical Kinetic Mechanisms:

**Diesel Mechanism:** Typically includes a detailed set of reactions representing the oxidation of long-chain hydrocarbons. Mechanisms like the n-heptane mechanism are often used as surrogates for diesel.

**Hydrogen Mechanism:** A simplified mechanism with fewer reactions, focusing on the high reactivity and fast kinetics of hydrogen. Common mechanisms include the GRI-Mech 3.0.

**Biofuel Mechanism:** Varies based on the type of biofuel. For biodiesel, mechanisms often include methyl esters representing fatty acid methyl esters (FAME). For ethanol, detailed mechanisms capturing the oxidation of  $C_2H_5OH$  are used.

### 4. Combustion Characteristics

#### 4.1. Enhanced Combustion Efficiency:

**Hydrogen Addition:** Hydrogen's high diffusivity and flame speed enhance the combustion process, leading to more complete fuel oxidation and higher peak temperatures.

**Biofuel Addition:** Biofuels, particularly those with high oxygen content like biodiesel, improve combustion efficiency by providing additional

oxygen for the combustion process, reducing soot formation.

#### 4.2. Combustion Phasing:

**Advanced Combustion Phasing:** The addition of hydrogen tends to advance the start of combustion due to its lower ignition delay, resulting in a more efficient combustion process.

**Effect of Biofuels:** The presence of biofuels can either advance or delay combustion phasing depending on their chemical composition and reactivity.

#### 5. Engine Performance

##### 5.1. Brake Thermal Efficiency (BTE):

**Improved Efficiency:** Studies show that blending hydrogen with diesel generally improves BTE due to better combustion efficiency and higher energy content of hydrogen.

**Biofuel Impact:** Biofuels can enhance BTE by promoting cleaner combustion and reducing heat losses, although the effect varies with the type of biofuel used.

##### 5.2. Brake Specific Fuel Consumption (BSFC):

**Reduction in BSFC:** Hydrogen addition typically reduces BSFC due to its higher energy content and better combustion characteristics.

**Biofuel Contribution:** The effect of biofuels on BSFC is mixed; while some biofuels like biodiesel can reduce BSFC by enhancing combustion

efficiency, others like ethanol may increase it due to lower energy density.

#### 6. Emissions

##### 6.1. Nitrogen Oxides (NO<sub>x</sub>) Emissions:

**Increased NO<sub>x</sub> with Hydrogen:** The higher combustion temperatures associated with hydrogen addition often lead to increased NO<sub>x</sub> emissions. However, the extent of the increase depends on the blend ratio and combustion control strategies.

**Biofuel Impact:** Biofuels can help mitigate NO<sub>x</sub> emissions due to their lower adiabatic flame temperature and higher oxygen content, which promotes more complete combustion at lower temperatures.

##### 6.2. Particulate Matter (PM) Emissions:

**Reduction in PM:** Both hydrogen and biofuels contribute to reducing PM emissions. Hydrogen promotes cleaner combustion with minimal soot formation, while biofuels, especially oxygenated ones like biodiesel, reduce soot precursors and enhance oxidation of soot particles.

##### 6.3. Carbon Monoxide (CO) and Hydrocarbon (HC) Emissions:

**Reduction in CO and HC:** Hydrogen addition significantly reduces CO and HC emissions due to its cleaner burning properties and higher reactivity, which promote complete combustion. Biofuels also contribute to lower CO and HC emissions by

providing additional oxygen and reducing incomplete combustion.

## 7. Conclusion

The numerical investigation of multi-fuel (diesel, hydrogen, and biofuel) combustion in CI engines using CFD provides valuable insights into the potential benefits and challenges associated with this approach. The key findings from recent studies indicate that multi-fuel blends can significantly enhance engine performance and reduce emissions when optimized properly.

### Key Takeaways

#### 7.1. Improved Combustion Efficiency:

The addition of hydrogen and biofuels to diesel improves combustion efficiency due to hydrogen's high reactivity and the oxygen content in biofuels, leading to more complete fuel oxidation.

This results in higher brake thermal efficiency (BTE) and lower brake specific fuel consumption (BSFC), contributing to better overall engine performance.

#### 7.2. Emissions Reduction:

Hydrogen and biofuels help reduce particulate matter (PM), carbon monoxide (CO), and hydrocarbon (HC) emissions due to their cleaner burning properties.

However, managing NO<sub>x</sub> emissions remains a challenge with hydrogen addition, requiring

advanced combustion control and after treatment technologies.

#### 7.3. Optimal Fuel Blends:

The optimal ratios of diesel, hydrogen, and biofuels can vary, but blends that balance high energy content, efficient combustion, and reduced emissions are most promising.

Multi-fuel blends leveraging the strengths of each fuel type can achieve substantial improvements in engine performance and emissions control.

#### 7.4. Technological and Economic Challenges:

Issues such as hydrogen storage and handling, biofuel stability, and the need for engine modifications pose significant challenges. The economic viability of hydrogen and biofuels requires further advancements in production, storage, and distribution technologies, as well as supportive policies and incentives.

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