

Numerical Investigation of Multi-Fuel (Diesel + Hydrogen + Biofuel) Combustion in CI Engines Using CFD

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Abstract

This research paper presents a detailed numerical investigation of multi-fuel combustion involving diesel, hydrogen, and biofuel in compression ignition (CI) engines using Computational Fluid Dynamics (CFD). The study aims to understand the synergetic effects of these fuel blends on combustion characteristics, engine performance, and emissions. By leveraging advanced CFD techniques, this work explores the potential of optimizing multi-fuel blends to achieve cleaner and more efficient combustion in CI engines.

Keywords: *CFD, CI engine, Biofuel, Mixed Fuel, Diesel, Computational Fluid Dynamics*

Introduction

The internal combustion engine (ICE) sector faces increasing challenges due to stringent emissions regulations and the need for sustainable energy solutions. The integration of alternative fuels such as hydrogen and biofuels with conventional diesel presents a viable pathway towards reducing emissions and enhancing fuel efficiency. This study focuses on the numerical simulation of multi-fuel combustion in CI engines using CFD to elucidate the complex interactions between different fuel components and their impact on engine performance.

Background and Motivation

1. Environmental Concerns: Reducing greenhouse gas emissions and particulate matter is critical for environmental protection.

2. Sustainability: Utilizing biofuels supports renewable energy initiatives and reduces reliance on fossil fuels.

3. Combustion Efficiency: Hydrogen's high reactivity can improve combustion efficiency, while biofuels offer cleaner combustion.

Methodology

Computational Fluid Dynamics (CFD) Framework

CFD is a powerful tool for investigating the complex phenomena associated with multi-fuel combustion in CI engines. This section details the methodology used in the CFD analysis, including the governing equations, turbulence modeling, chemical kinetics, and the setup of simulations for multi-fuel combustion.

Governing Equations

The foundation of CFD modeling lies in solving the governing equations for fluid dynamics, heat transfer, and chemical reactions. These equations are:

1. Continuity Equation: Ensures mass conservation in the flow field.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

where ρ is the density and \mathbf{u} is the velocity vector.

2. Navier-Stokes Equations: Govern the momentum conservation in the fluid.

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \mathbf{S}_{\text{momentum}}$$

where p is the pressure, μ is the dynamic viscosity, and S_{momentum} represents the source terms.

3. Energy Conservation Equation: Describes the conservation of energy in the system.

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = \nabla \cdot (k \nabla T) + S_{\text{energy}}$$

where E is the total energy, k is the thermal conductivity, T is the temperature, and S_{energy} represents the source terms, including heat release from combustion.

4. Species Transport Equations: Govern the conservation of individual chemical species.

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (D_i \nabla Y_i) + \dot{\omega}_i$$

where Y is the mass fraction of species D is the diffusion coefficient, and ω is the reaction rate of species i .

Turbulence Modeling

Accurate turbulence modeling is crucial for capturing the mixing and combustion processes in CI engines. Several turbulence models are available, with the most commonly used being:

1. k- ϵ Model: A two-equation model that solves transport equations for the turbulent kinetic energy (k) and its dissipation rate (ϵ).

$$\frac{\partial(\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} k) = \nabla \cdot \left(\frac{\mu_t}{\sigma_k} \nabla k \right) + G_k - \rho \epsilon$$

$$\frac{\partial(\rho \epsilon)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \epsilon) = \nabla \cdot \left(\frac{\mu_t}{\sigma_\epsilon} \nabla \epsilon \right) + C_1 \frac{\epsilon}{k} G_k - C_2 \rho \frac{\epsilon^2}{k}$$

where G_k is the generation of turbulent kinetic energy due to mean velocity gradients, and μ_t is the turbulent viscosity.

2. k- ω Model: Another two-equation model that solves for the turbulent kinetic energy (k) and the specific dissipation rate (ω).

$$\frac{\partial(\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} k) = \rho \beta^* k \omega + \nabla \cdot ((\mu + \sigma_k \mu_t) \nabla k)$$

$$\frac{\partial(\rho \omega)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \omega) = \alpha \frac{\omega}{k} P_k - \beta \rho \omega^2 + \nabla \cdot ((\mu + \sigma_\omega \mu_t) \nabla \omega)$$

where P_k is the production of turbulent kinetic energy, and α , β , β^* , σ_k , and σ_ω are model constants.

3. Large Eddy Simulation (LES): A more advanced approach that resolves large turbulent structures and models the smaller scales using a sub-grid scale (SGS) model.

Chemical Kinetics

The accurate simulation of combustion processes requires detailed chemical kinetics. The chemical reaction mechanisms for diesel, hydrogen, and biofuels are incorporated into the CFD model to capture the combustion behavior accurately.

1. Diesel Combustion Mechanism: Typically includes a large number of hydrocarbon species and reactions to represent the complex oxidation process of diesel fuel.

2. Hydrogen Combustion Mechanism: Simpler than diesel, involving fewer species and reactions, but requires accurate representation of the high reactivity and fast kinetics of hydrogen.

3. Biofuel Combustion Mechanism: Varies depending on the type of biofuel (e.g., biodiesel, ethanol) and includes specific reactions relevant to the biofuel's chemical structure.

Simulation Setup

The simulation setup involves defining the engine geometry, boundary conditions, initial conditions, and operating parameters to replicate real engine conditions.

- 1. Engine Geometry:** A 3D model of the engine cylinder, including the piston, cylinder head, and intake/exhaust ports, is created.
- 2. Boundary Conditions:** Appropriate boundary conditions for pressure, temperature, and velocity are applied at the inlet and outlet of the cylinder.
- 3. Initial Conditions:** The initial distribution of pressure, temperature, and species concentrations within the cylinder is specified.
- 4. Operating Parameters:** Engine speed, load, fuel injection timing, and equivalence ratio are defined based on the specific operating conditions being studied.

Simulation

The simulation phase involves setting up, running, and analyzing CFD simulations to study the combustion characteristics of multi-fuel blends in CI engines. This process includes defining the computational domain, mesh generation, setting boundary and initial conditions, specifying operating parameters, and post-processing the results.

Computational Domain and Mesh Generation

1. Engine Geometry: A detailed 3D model of the engine cylinder is created, including the piston, cylinder head, intake, and exhaust ports. The geometry is prepared using CAD software and imported into the CFD software.

2. Mesh Generation: The computational domain is discretized into small control volumes (cells) using a suitable meshing technique. A fine mesh is used in regions with high gradients (e.g., near the fuel injection and combustion zones) to capture the

detailed flow and combustion processes accurately. The mesh quality is ensured by checking for skewness, aspect ratio, and other mesh metrics.

Boundary and Initial Conditions

- 1. Boundary Conditions:** Appropriate boundary conditions are applied to the computational domain:
 - Inlet Boundary:** Specified mass flow rate, temperature, and species concentrations of the intake air-fuel mixture.
 - Outlet Boundary:** Pressure outlet boundary condition with specified pressure and temperature.
 - Wall Boundaries:** No-slip boundary condition with specified wall temperature for the cylinder walls, piston, and cylinder head.

2. Initial Conditions: The initial conditions for pressure, temperature, velocity, and species concentrations within the cylinder are set based on the engine's operating conditions. Typically, the initial conditions are specified at the start of the compression stroke.

Operating Parameters

- 1. Engine Speed and Load:** The engine speed (RPM) and load conditions are defined based on the specific operating scenario being studied.
- 2. Fuel Injection Parameters:** The injection timing, duration, and rate are specified for each fuel component (diesel, hydrogen, and biofuel). Multi-fuel injection strategies may involve simultaneous or sequential injection of different fuels.
- 3. Equivalence Ratio:** The overall equivalence ratio (fuel-to-air ratio) is set to represent the desired combustion stoichiometry.

Running the Simulation

The CFD simulation is run using a suitable solver that handles compressible reactive flows. The solver iteratively solves the governing equations for fluid

flow, heat transfer, and chemical reactions within the computational domain.

1. Time Step Selection: A suitable time step is chosen to ensure numerical stability and accuracy. Adaptive time stepping may be used to handle rapid changes in the combustion process.

2. Convergence Criteria: The simulation is monitored for convergence by checking residuals of the governing equations and ensuring that key parameters (e.g., pressure, temperature, and species concentrations) reach steady values.

3. Parallel Computing: High-performance computing (HPC) resources may be utilized to speed up the simulation by running it in parallel on multiple processors.

Post-Processing and Analysis

The results of the CFD simulation are post-processed to analyze the combustion characteristics, engine performance, and emissions.

1. Combustion Characteristics:

Temperature Distribution: Analyze the temperature profiles within the cylinder to identify peak temperatures and regions of intense combustion.

Pressure Variation: Study the in-cylinder pressure variation over the engine cycle to understand the combustion dynamics.

Species Concentrations: Examine the distribution of key species (e.g., CO, CO₂, NO_x, unburned hydrocarbons) to evaluate the completeness of combustion and formation of pollutants.

2. Engine Performance:

Brake Thermal Efficiency (BTE): Calculate BTE to assess the efficiency of converting fuel energy into mechanical work.

Brake Specific Fuel Consumption (BSFC): Evaluate BSFC to determine the fuel economy of the engine.

3. Emissions Analysis:

NO_x Emissions: Quantify NO_x emissions to understand the impact of combustion temperature and fuel composition.

Particulate Matter (PM): Analyze PM emissions to evaluate the effectiveness of multi-fuel blends in reducing soot formation.

CO and HC Emissions: Assess CO and unburned hydrocarbon emissions to gauge the completeness of combustion.

Validation

The simulation results are validated against experimental data to ensure the accuracy and reliability of the CFD model. Key parameters such as pressure traces, temperature profiles, and emissions data are compared with experimental measurements.

Sensitivity Analysis

A sensitivity analysis is performed to study the impact of various parameters (e.g., fuel blend ratio, injection timing, equivalence ratio) on the combustion process and engine performance. This helps in identifying optimal conditions for achieving cleaner and more efficient combustion.

Fuel Blend Ratios and Optimization

1. Optimal Blend Ratios:

Diesel-Hydrogen: Studies suggest that blend ratios around 80% diesel - 20% hydrogen or 70% diesel - 30% hydrogen provide a good balance between improved efficiency and manageable NO_x emissions.

Diesel-Biofuel: Ratios such as 80% diesel - 20% biodiesel or 70% diesel - 30% ethanol have been shown to enhance combustion efficiency and reduce

emissions without significantly affecting engine performance.

2. Multi-Fuel Blends:

Synergistic Effects: Combining diesel, hydrogen, and biofuels can leverage the benefits of each fuel type. For example, a blend of 70% diesel - 15% hydrogen - 15% biodiesel can achieve high efficiency and low emissions by optimizing the combustion characteristics of each component.

Combustion Stability: Multi-fuel blends generally improve combustion stability due to the combined effects of different fuel properties, leading to more robust and reliable engine performance.

Sensitivity to Operating Conditions

1. Injection Timing:

Advanced Timing: Advancing the injection timing can enhance the benefits of hydrogen addition by further reducing ignition delay and promoting faster combustion. However, it may also increase NOx emissions.

Biofuel Sensitivity: Biofuels' impact on combustion is sensitive to injection timing, with optimal timing varying depending on the specific biofuel used.

2. Equivalence Ratio:

Lean Combustion: Operating under lean conditions (lower equivalence ratios) generally favors the benefits of hydrogen addition by reducing NOx emissions and enhancing combustion efficiency.

Rich Combustion: Higher equivalence ratios can increase CO and HC emissions, but the presence of biofuels can mitigate these effects due to their higher oxygen content.

Challenges

1. Fuel Storage and Handling:

Hydrogen Storage: Hydrogen requires high-pressure tanks or cryogenic systems for storage, posing challenges in terms of safety, infrastructure, and cost.

Biofuel Stability: Biofuels, particularly biodiesel, can have issues with oxidation stability and cold flow properties, requiring additives or modifications for consistent performance.

2. Combustion Control:

Ignition Delay and Phasing: Managing the ignition delay and combustion phasing in multi-fuel blends is complex due to the different ignition properties of diesel, hydrogen, and biofuels.

Knock Control: High reactivity fuels like hydrogen can cause knocking, especially at higher blend ratios, necessitating advanced control strategies.

3. Emissions Management:

NOx Emissions: While hydrogen can reduce PM, it often increases NOx emissions. Balancing the reduction of both NOx and PM simultaneously is a significant challenge.

Unburned Hydrocarbons (UHC): Biofuels can increase UHC emissions under certain conditions, particularly if not fully vaporized or mixed properly.

4. Engine Modifications:

Injection Systems: Existing fuel injection systems may need modifications to handle multi-fuel blends, including different injectors or injection strategies.

Materials Compatibility: Components in the fuel system must be compatible with biofuels, which can be more corrosive or have different lubrication properties compared to diesel.

5. Economic Viability:

Cost of Hydrogen: The production, storage, and distribution of hydrogen remain expensive, which can be a barrier to its widespread adoption.

Biofuel Production: Sustainable and cost-effective production of biofuels at scale is necessary to ensure their economic viability as a diesel substitute.

Future Directions

1. Advanced Combustion Technologies:

Dual-Fuel Injection Systems: Develop advanced dual-fuel injection systems capable of precise control over diesel, hydrogen, and biofuel injection to optimize combustion efficiency and emissions.

Low-Temperature Combustion (LTC): Explore LTC strategies such as homogeneous charge compression ignition (HCCI) or reactivity-controlled compression ignition (RCCI) for better emissions control and efficiency with multi-fuel blends.

2. Hydrogen Production and Storage Innovations:

Green Hydrogen Production: Invest in renewable energy-based hydrogen production methods (e.g., electrolysis using solar or wind power) to reduce the carbon footprint and cost of hydrogen.

Improved Storage Solutions: Research advanced hydrogen storage materials (e.g., metal hydrides, carbon nanotubes) that offer higher storage densities and safer handling.

3. Biofuel Development:

Second-Generation Biofuels: Focus on second-generation biofuels derived from non-food biomass, such as lignocellulosic feedstocks, to enhance sustainability and reduce competition with food crops.

Algae-Based Biofuels: Investigate the potential of algae-based biofuels, which can be produced using

non-arable land and have high lipid content for biodiesel production.

4. Engine and Fuel System Optimization:

Adaptive Control Systems: Develop adaptive engine control systems that can dynamically adjust parameters (e.g., injection timing, fuel ratio) based on real-time feedback to optimize performance and emissions.

Materials Research: Innovate materials for engine components that can withstand the unique properties of multi-fuel blends, such as higher temperatures and different chemical compositions.

5. Emissions Reduction Technologies:

Exhaust Aftertreatment Systems: Enhance aftertreatment technologies, such as selective catalytic reduction (SCR) for NO_x control and particulate filters for PM reduction, to complement the benefits of multi-fuel combustion.

Catalyst Development: Research advanced catalysts that can effectively reduce emissions from biofuel combustion, particularly for UHC and CO.

6. Economic and Policy Support:

Subsidies and Incentives: Implement subsidies and incentives for hydrogen and biofuel production and usage to make them more competitive with traditional fuels.

Infrastructure Development: Invest in infrastructure for hydrogen refueling stations and biofuel distribution networks to support widespread adoption.

7. Comprehensive Lifecycle Analysis:

Environmental Impact Assessment: Conduct comprehensive lifecycle analyses to assess the overall environmental impact of multi-fuel blends, from production to combustion, ensuring sustainability and reducing greenhouse gas emissions.

CH₄ combustion at main combustion stage.

Figure 1 shows the simulated evolution of n-heptane spray, the distribution of temperature, ER, and CH₄ in a cut-plane in the middle of the injection spray for the 25NG case. In this research, the ER is calculated using the concentration of fuel and O₂ without accounting for CO₂ and H₂O formed through the combustion of the pilot and CH₄. With the development of the spray plume, the ER within the n-heptane spray plume is found to first gradually increase accompanied by the injection of pilot fuel but then decrease due to the atomization and vaporization of n-heptane and mixing with the CH₄-air mixture.

The continued increase in ER within pilot fuel spray, especially after the consumption of n-heptane, is due to the consumption of O₂ during the combustion process of n-heptane and CH₄ within the spray plume. The concentration of CH₄ and the temperature inside the spray are noted to increase from -2.5 to 0.1 °crank angle (CA) after top dead center (ATDC). This is due to the formation of CH₄ during the oxidation of n-heptane.

Accordingly, not all of the CH₄ present outside the n-heptane spray plume can be burned due to the lack of flame propagation. With the combustion of CH₄ in the rich mixture featuring ER>1, the ER value would further increase due to the consumption of O₂. In comparison, the ER of the lean fuel mixture (ER<1) would gradually decrease to zero (complete combustion) with the consumption of fuel as there is excess O₂ present. The temperature distribution shows that ignition is first observed at the periphery of the n-heptane plume where n-heptane and methane-air mixture are sufficiently mixed. n-heptane Temperature Equivalent ratio CH₄ From top to bottom: -2.5°, 0.1°, 4.3° CA ATDC.

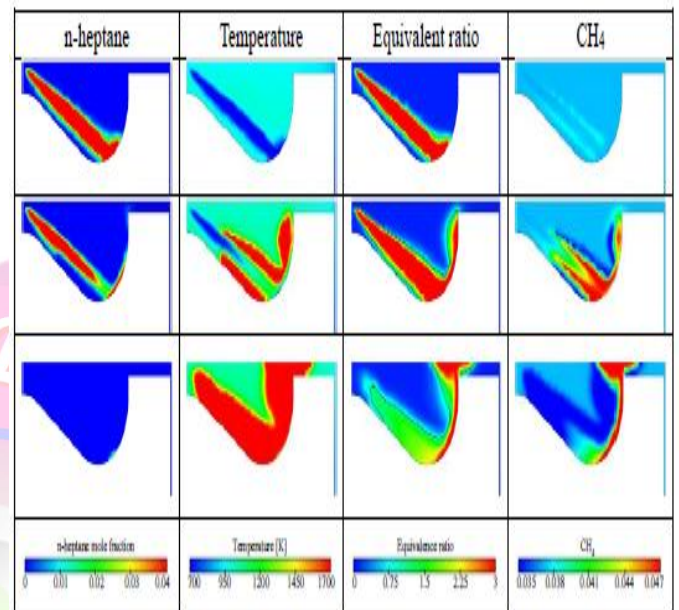


Figure 1 The evolution of spray plume, distribution of temperature, equivalent ratio, and molar fraction of CH₄ during n-heptane injection and ignition process. Case: 25NG.

Results and Discussion

Combustion Characteristics

- 1. Ignition Delay:** The addition of hydrogen reduces ignition delay due to its higher reactivity, while biofuels exhibit a longer ignition delay compared to pure diesel.
- 2. Combustion Duration:** Biofuels increase the combustion duration due to their lower volatility, while hydrogen enhances the combustion process, resulting in a shorter combustion duration.
- 3. Combustion Temperature:** Multi-fuel blends achieve higher peak temperatures, improving thermal efficiency but necessitating careful control to mitigate NO_x formation.

Emission and Engine Performance

This section presents a detailed analysis of the effects of multi-fuel (diesel + hydrogen + biofuel) combustion on emissions and engine performance in CI engines. The findings are based on recent studies and CFD simulations, highlighting the

interplay between fuel blends, combustion dynamics, and their impact on overall engine efficiency and emissions.

Emission Analysis

1. Nitrogen Oxides (NOx) Emissions:

Hydrogen Addition: Hydrogen typically increases NOx emissions due to higher peak combustion temperatures. The rapid combustion of hydrogen results in elevated in-cylinder temperatures, promoting NOx formation through the thermal NOx mechanism.

Biofuel Impact: The addition of biofuels like biodiesel, which have lower adiabatic flame temperatures compared to diesel, can help mitigate NOx emissions. Biofuels' oxygen content also supports more complete combustion at lower temperatures.

Optimization: Strategies such as exhaust gas recirculation (EGR) and retarded injection timing can be employed to manage NOx emissions when using hydrogen-diesel blends.

2. Particulate Matter (PM) Emissions:

Reduction with Hydrogen: Hydrogen addition significantly reduces PM emissions due to its clean-burning nature and lack of carbon content, which eliminates soot formation.

Biofuel Benefits: Biofuels, especially oxygenated ones like biodiesel, also reduce PM emissions by enhancing soot oxidation during combustion. The additional oxygen content in biofuels promotes more complete fuel oxidation, lowering soot precursors.

Synergistic Effects: Combining hydrogen and biofuels with diesel can achieve substantial reductions in PM emissions, leveraging the clean-burning characteristics of hydrogen and the oxidation-promoting properties of biofuels.

3. Carbon Monoxide (CO) and Hydrocarbon (HC) Emissions:

Hydrogen Impact: The high reactivity and fast flame speed of hydrogen lead to more complete combustion, significantly reducing CO and HC emissions. Hydrogen's clean-burning properties result in fewer incomplete combustion products.

Biofuel Contribution: Biofuels can further reduce CO and HC emissions due to their higher oxygen content, which supports more complete combustion. However, the specific impact varies with the type of biofuel and its blend ratio with diesel.

Optimization: Optimal blend ratios and injection strategies can minimize CO and HC emissions while maintaining efficient combustion.

Engine Performance Analysis

1. Brake Thermal Efficiency (BTE):

Hydrogen Enhancement: Hydrogen addition generally improves BTE due to its high energy content and efficient combustion characteristics. The rapid and complete combustion of hydrogen leads to better energy conversion.

Biofuel Impact: Biofuels can enhance BTE by promoting cleaner combustion and reducing heat losses. For example, biodiesel's higher oxygen content can improve combustion efficiency, while ethanol's high octane number can prevent knocking.

Combined Effects: Using a combination of hydrogen, biofuels, and diesel can optimize BTE by leveraging the strengths of each fuel. Blends that balance high energy content, clean combustion, and optimal ignition properties can achieve the best efficiency.

2. Brake Specific Fuel Consumption (BSFC):

Hydrogen Reduction: Hydrogen typically reduces BSFC due to its higher energy content per unit mass compared to diesel. The improved combustion

efficiency with hydrogen addition also contributes to lower fuel consumption.

Biofuel Variability: The impact of biofuels on BSFC varies. Biodiesel can reduce BSFC by improving combustion efficiency, while ethanol might increase it due to lower energy.

Experimental setup and numerical simulation model

Experimental set-up

The experiments were conducted in a single cylinder, 4-valve, caterpillar diesel engine with a compression ratio of 16.25, bore of 137.2 mm, and stroke of 165.1 mm. The engine test cell was configured to simulate the operation of a turbocharged heavy-duty diesel engine. The detailed specification of the engine, dynamometer, data acquisition system, and exhaust gas analyzer can be found in the literature [33]. In this research, NG was added to the intake air using a port-fuel NG injector installed between the intake surge tank and intake valve. The pilot diesel was directly injected into the cylinder using a common-rail fuel injection system at 525 bar. The diesel injector has 6 injection holes of diameter 0.23 mm and is installed at the center of the cylinder head. The injection spray angle was 65°. In this research, the engine was operated at an engine speed of 910 rpm, and a brake mean effective pressure (bmepp) of 4.05 bar, a typical low load operation condition featured with low methane combustion efficiency. The gaseous fuel used was pipeline natural gas consisting of 95.80% methane, 2.34% ethane, 0.19% propane, 0.98% N₂, 0.64% CO₂ and traceable high hydrocarbons [33].

The simulation started from the intake valve closing (IVC) with the assumed homogeneous mixture of natural gas, air, and residual gas and completed at the exhaust valve opening (EVO). The pressure, temperature, and composition of bulk mixture were calculated with the cylinder pressure and

temperature at the end of the exhaust stroke. The mass and concentration of the air-fuel mixture consumed each cycle was calculated using experimental data. The simulation data was processed to examine the mechanism for methane to survive the main and post-combustion process, the spatial distribution of methane in-cylinder, and the percentage of methane consumed in each combustion stage.

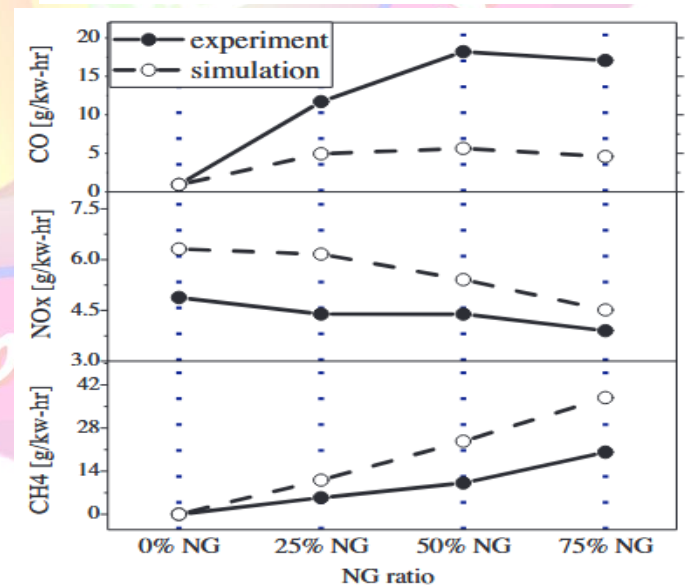
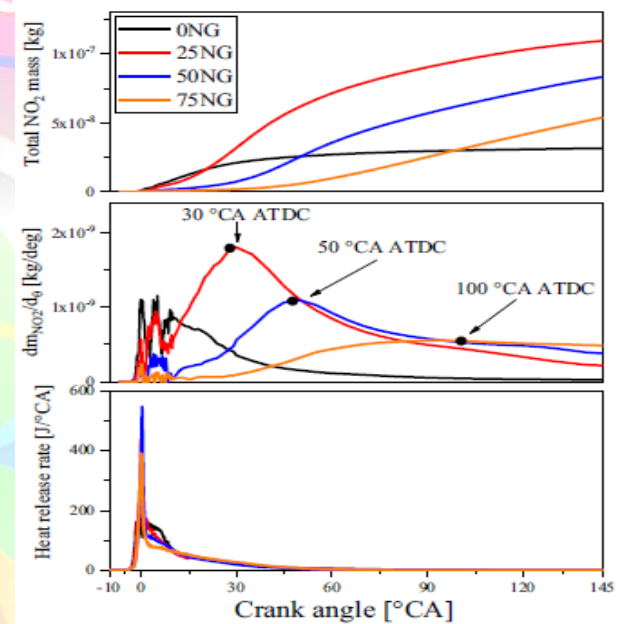


Figure 2 Comparison of simulated NO_x, NO₂, NO emission and NO₂/NO_x mass ratio with experimental data

Discussion

The simulation work conducted in this research reveals the combustion of methane in a dual fuel engine, the important role of post-combustion oxidation in burning the methane surviving the main combustion process, and the spatial distribution of the unburned methane in-cylinder. The optimization of the engine aiming to enhance the combustion of methane in a dual fuel engine should focus on the following aspects:

(ii) Increasing the ignition delay time period to allow for enough time for the atomization, vaporization of pilot fuel, and its mixing with bulk gas prior to the auto-ignition of the pilot fuel vapor. This can be achieved through optimizing fuel injection strategies such as using multiple-fuel injection pulses such as adding a mini-pilot injection pulse prior to the main injection pulse of pilot fuel.

(2) Enhancing the movement of the hot bulk gas toward the cold unburned methane mixture, especially the movement of hot combustion products toward the center of the cylinder, which requests a better design of the piston bowl geometry. The mixing of the combustion products with the unburned premixed mixture should occur early in the expansion process when the temperature of the hot combustion products is still sufficiently high to oxidize the unburned methane.

Conclusion

This research numerically investigates the combustion process and exhaust emissions from a NG-diesel dual fuel engine using CFD model CONVERGE coupled with a reduced PRF chemistry. A post-processing tool has been developed to calculate, analyze, and visualize the instantaneous ROP of key species in each cell with the known temperature, pressure, and species concentration exported by the CFD model. The ROP data is post-processed to derive the key reactions dominating the formation of CO, NO₂ and the consumption of CH₄ in a NG-diesel dual fuel engine. Based on the simulation work conducted in this research, the following conclusions can be drawn:

□ The combustion of CH₄ in a NG-diesel dual fuel engine at low loads was dominated by the combustion of the pilot fuel, the relative volumetric ratio of pilot fuel vapor over the total volume, the movement of the hot combustion products towards the unburned mixture, and the mixing of the hot

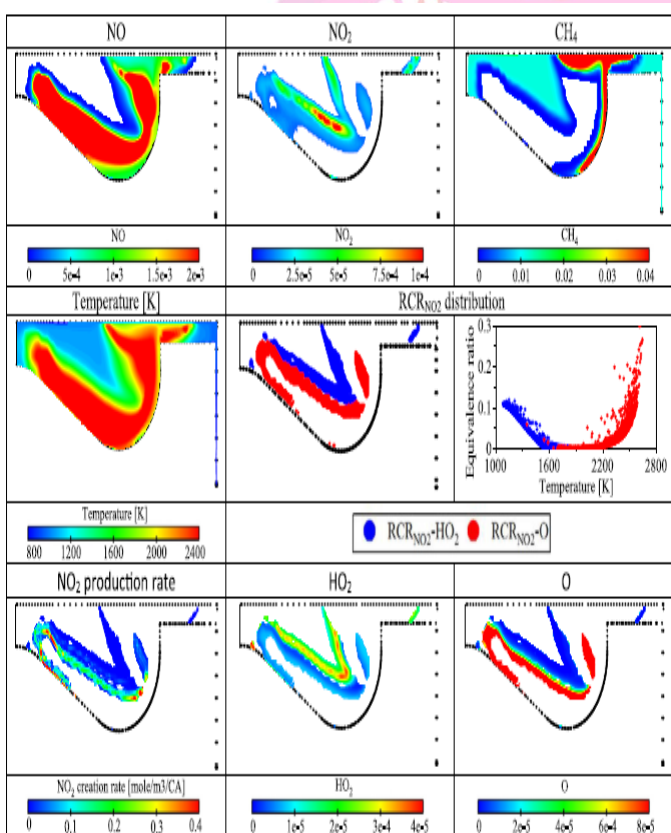


Figure 3 Temperature, RCR NO₂ distribution in cut-plane and phi-T diagram, CH₄, NO, NO₂, HO₂, and O molar fraction, NO₂ production rate at Region 1, CA50, 7 °CA ATDC, 25NG case.

(1) increasing the relative volumetric ratio of bulk gas mixed with vapors of the pilot fuel. This can be achieved through

(i) modifying the design of the fuel injector such as increasing the size or volume of pilot fuel spray plume which can be achieved through the adjusting the spray angle, number of injection holes, and diameter of injector holes;

combustion products with the unburned CH₄-air mixture.

□ The spray plume of the pilot fuel injected into the cylinder produced a high velocity field of the bulk gas under the guidance of the piston bowl shape, which helped the mixing of the hot combustion products with the unburned CH₄ and contributes most to CH₄ consumption during the combustion process. The main 143 combustion process consumed 43% to 53% of the total CH₄ in cylinder.

□ The post-combustion oxidation of CH₄ occurred in the interface between the hot combustion products and the unburned pre-mixed NG-air mixture, which increased the temperature of CH₄ to that needed for its oxidation. The post-combustion process consumes 17% to 29% CH₄.

□ The unburned CH₄ observed at EVO was located mainly at the center of the cylinder. The portion of CH₄ present at the boundary layer near the cylinder liner was relatively small. The total CH₄ left unburned at EVO was 27 to 35% of the intake CH₄ at the low load case simulated

□ The optimization of dual fuel engine design, operation and fuel injection strategies aiming to minimizing CH₄ emissions should focus on those capable of increasing the relative volume of the pilot fuel vapor or its combustion products or increasing the chance to mix with hot combustion products early in the expansion process when the temperature of the combustion products is still high.

□ The increased NO₂ emitted from NG-diesel dual fuel engine was mainly formed in the interface region between the hot NO-containing combustion products and the cool, unburned CH₄-air mixture during the post-combustion expansion process. The oxidation of the CH₄ provided the HO₂ needed for the conversion from NO to NO₂. The low NO₂ emissions from diesel engine might be due to lack of HO₂ formed during post-combustion expansion process. 144

□ The NO₂ formed within pilot fuel spray during the early combustion process was converted to NO due to the high temperature of the combustion products, and the complete consumption of HO₂ present with NO after the complete oxidation of the local CH₄ and n-heptane. The NO₂ observed at EVO was formed mainly in the post combustion expansion process.

□ The HO₂ needed for the conversion from NO to NO₂ was formed during the CH₄ oxidation process through the reaction path: CH₄→CH₃→CH₂O→HCO→HO₂. The reaction 54: HCO+O₂=HO₂+CO provided 98% of the HO₂ formed in the particular case examined in this research. The backward reaction of OH+NO₂=NO+HO₂ consumed 34% of HO₂ for the conversion from NO to NO₂.

□ The NO to NO₂ conversion reaction was dominated by the temperature of the mixture consisting of NO, CH₄, O₂, etc. In comparison, the impact of ER of gaseous fuel or concentration of CH₄ on the conversion reaction rate factor was negligible.

□ The distribution of NO and NO₂ in the ER-T diagram confirmed that the NO₂ emitted from a NG-diesel dual fuel engine was mainly formed and distributed in the mixture with a relatively low temperature. This ruled out the possibility for the NO₂ formed in the hot combustion zone of the pilot fuel to survive until EVO.

□ The NO₂ in a NG-diesel dual fuel engine can be formed in the RCRNO₂-O and RCRNO₂-HO₂ regions. The RCRNO₂-O region represents the formation of NO₂ in high-temperature combustion products during the main combustion stage of pilot fuel. The RCRNO₂-HO₂ region represents the interface between the hot 145 NO-containing combustion products and the cool CH₄-containing unburned CH₄-air mixture. The increased NO₂ emissions from NG-diesel dual fuel engines are mainly formed in the RCRNO₂-HO₂ region.

□ The HO₂ radical required for NO-NO₂ conversion in the RCRNO₂-HO₂ region is produced by the reaction pathway: CH₄→CH₃→CH₂O→HCO→HO₂. The presence of the RCRNO₂-HO₂ region contributes to the significantly increased NO₂ emissions from a NG-diesel dual fuel engine compared to a traditional diesel engine. The unburned CH₄/air that survives the main combustion stage provides the CH₄ source for the production of HO₂ leading to the formation of more NO₂ in NG-diesel dual fuel engines than traditional diesel engines.

□ The O radical required for NO-NO₂ conversion in the RCRNO₂-O region is produced by the reaction pathway: HCO→H→O, through reaction R17 and R18 with HCO produced during the oxidation process of n-Heptane noted as C₇H₁₅→CH₂O→HCO→H→O→NO₂. The examination of the RRC reveals that the key factor causing R17 and R18 to dominate HCO and H radical consumption is the high temperature. Therefore, the RCRNO₂-O region is featured with high temperature and the presence of O₂. Meanwhile, the high temperature can promote the destruction of NO₂ to NO by R3 and R4. As a result, the NO₂ concentration in the RCRNO₂-O region is lower than that in the RCRNO₂-HO₂ region. In addition, the NO₂ eventually emitted from dual fuel engines is mainly formed in the RCRNO₂-HO₂ region.

□ The NO₂ emission from a NG-diesel dual fuel engine is determined by the total volume of RCRNO₂-HO₂ region and R1 reaction rate in the RCRNO₂-HO₂ region. Compared with the 25NG case, the 50NG case has comparable RCRNO₂-HO₂ region volume but significantly lower R1 reaction rate due to the combined effect of various factors such as local temperature, CH₄ concentration, and interaction between hot NO-containing combustion products and cool CH₄/air mixture. The volume and R1 reaction rate of the

RCRNO₂-HO₂ region observed in the 50NG and 75NG cases are both lower than the 25NG case. □ The CO in Region-H was mainly produced by incomplete combustion of the diesel fuel during the main combustion stage. In comparison, the CO in Region-L of the 25NG case was produced by slow oxidation of lean diesel fuel, and oxidation of NG when mixed with the combustion products of lean diesel-air mixture formed during the main combustion process.

□ The CO formation/consumption in Region-H of the diesel-only and NG-diesel dual fuel combustion mode was dominated by the intense competition between the forward and reverse reaction HCO=H+CO at the interface between the RDRCO-R1 region and the RCRCO-R1 region. The consumption of CO formed in Region-H was dominated by reaction CO+OH=CO₂+H which is affected by the entrainment of O₂-containing mixtures into the CO-containing region. The CO produced during the main combustion stage was consumed through CO→HCO→CO→CO₂+H→OH. The OH radicals enhances the CO consumption during the post-combustion expansion process.

□ The CO formation/consumption mechanism in Region-H was similar for both diesel engine combustion and NG-diesel dual fuel combustion modes. The addition of NG to intake air weakened the reactivity in region-H by reducing the 147 temperature and concentration of the active radicals such as H and OH, leading to the weakened reaction loop in the RDRCO-R2 region. Therefore, the CO formation or concentration in Region-H for dual fuel mode was higher than that for diesel combustion mode.

□ The CO formation/consumption mechanism in Region-L for the diesel only mode and dual fuel mode was significantly different. The CO in Region-L of diesel-only mode was produced by lean diesel-air fuel mixture near the spray

periphery. The CO formed was later consumed during the post combustion stage. However, the CO in Region-L of dual fuel mode was produced by co-oxidation of CH₄/air mixture and lean diesel-air mixture and its combustion products, which significantly increase the formation of CO in Region-L of dual fuel engine.

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