New Chemical Kinetics Mechanism for Simulation of Natural Gas/Hydrogen/Diesel Multi-fuel Combustion in Engines

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Abstract: Reactivity Controlled Compression Ignition (RCCI) stands out as a promising combustion method for the next wave of internal combustion engines, offering cleaner and more efficient operation, particularly in heavy-duty engines. A key approach within this strategy involves pairing diesel as the high reactivity fuel with natural gas (NG) as the low reactivity counterpart. Further optimization can be achieved by introducing hydrogen to replace portions of NG, thereby enhancing combustion quality while reducing greenhouse gas emissions. For accurate numerical simulation of engines employing this strategy, specialized chemical kinetics reaction mechanism tailored for internal combustion engines becomes essential. To facilitate computationally efficient 3-D Computational Fluid Dynamics (CFD) simulations, the mechanism has been reduced to include 60 species and 372 reactions, with N-heptane acting as a diesel fuel surrogate. This compact mechanism is optimized to align with experimental ignition delay time (IDT) data for N-heptane. The accuracy of the mechanism's predictions for IDT and laminar burning velocity (LBV) is validated using available experimental data. Furthermore, 3-D CFD and quasi-dimensional multi-zone engine simulations are performed with the new mechanism to validate engine operating parameters against experimental data.

Keywords: Diesel, Natural Gas, Simulation, Combustion, Engines, Mechanism

1. INTRODUCTION

Low-temperature combustion (LTC) is an advanced combustion concept for internal combustion engines that has attracted global attention in recent years. Among the LTC modes, Reactivity-Controlled Compression Ignition (RCCI), in particular, has demonstrated promising results in terms of reducing NOx emissions, brake thermal efficiency, and combustion phasing control when operated under certain conditions (Salahi et al., 2017). The unique operation of RCCI engines involves the intake of a low-reactivity fuel and the direct cylinder injection of a high-reactivity fuel (Hossein Fakhari et al., 2024). This process creates reactivity stratification, providing more control over the heat release rate. Recent advancements in RCCI engines have explored the use of alternative fuels and investigated combustion strategies to extend RCCI mode to higher loads (Fakhari et al., 2023). However, there is a recognized need for further enhancements in simulation models for these engines (Dwarshala et al., 2023).

Simulating combustion in internal combustion engines is crucial due to its impact on engine performance,emissions, and environmental regulations (Gössnitzer et al., 2022). Engine simulation methods have evolved significantly, with studies highlighting the use of simulation software to predict engine performance accurately.

Reliable and practical chemical kinetics are essential for the accuracy of modeling internal combustion engines (Kakoee et al., 2022). Vasudev et al. (Vasudev, Mikulski, et al., 2022) provide a detailed examination of chemical kinetics within the context of multi-zone models for low-temperature combustion engines. The review emphasizes the difficulties in striking a balance between computational efficiency and model complexity, and it suggests that developments in methods such as tabulated chemistry will lead to significant gains in simulation speed. Aziz et al. (Aziz et al., 2022) provided a comprehensive review of the impact of various fuels on the performance and emissions of RCCI engines, highlighting the benefits of using low-reactivity fuels like gasoline, natural gas, and alcohol-based fuels, as well as high-reactivity fuels like diesel and biodiesel. They explored fuel management strategies and the use of additives to enhance Ammonia and hydrogen has also attracted a lot of attention in marine and power plant applications (Salahi et al., 2022). Natural gas, with its great fuel economy, clean combustion characteristics, abundance, and comparatively low cost, is one of the most potential alternative fuels to meet ever-tougher pollution regulations (Gharehghani et al., 2023). The analysis of dual-fuel engines reveals that researchers need a more appropriate dual-fuel chemical kinetic mechanism involving diesel and natural gas (W. Zhang et al., 2019).

Optimizing the chemical kinetic mechanism for natural gas and diesel dual-fuel engines presents challenges, including the need for accurate prediction of combustion characteristics and emissions, understanding the impact of methane content on ignition delay, and ensuring mechanism accuracy across different fuel ratios (Aminian et al., 2023). Many researchers studied heavy substances as diesel fuel representatives. Guo et al. (Guo et al., 2021) generated a simplified mechanism (155 species, 645 reactions) for a diesel and natural gas dual-fuel RCCI engine, assuming n-hexadecane as diesel fuel. Using cross-reaction analysis, Liu et al. (Liu et al., 2021) developed a reduced combustion mechanism (150 species, 847 reactions) for a multi-component fuel mixture consisting of toluene, n-dodecane, methane, and methylcyclohexane. They validated it through testing against experimental ignition delay and flame speed data, ensuring its accuracy over a wide range of pressures, temperatures, and equivalence ratios. Zhou et al. (Zhou et al., 2023) introduced a new reduced mechanism (141 species, 739 reactions) for diesel (represented by n-dedocane) and natural gas combustion in HCCI applications. To create a compact model, they used simplification techniques such as directed relation graphs (DRG), DRG with error propagation (DRGEP), and sensitivity analysis.

It is generally acknowledged that the n-heptane oxidation processes accurately depict the properties of diesel fuel combustion in a simplified way (H. Wang et al., 2013). Recently, researchers have shown interest in utilizing reduced mechanisms in which n-heptane is the diesel fuel surrogate. Rahimi et al. (Rahimi et al., 2010) introduced a semi-detailed chemical kinetic mechanism (76 species, 464 reactions) for n-heptane and methane, optimized by a genetic algorithm. The mechanism has been continuously employed to simulate multi-fuel engines (Yin et al., 2024). Hockett et al. (Hockett et al., 2016) developed a reduced chemical mechanism (141 species, 709 reactions) known as CSU141 by combining two detailed mechanisms of n-heptane and natural gas (represented by a combination of methane, ethane, and propane). De Bellis et al. (De Bellis et al., 2022) modified this mechanism by adding a NOx sub-mechanism to develop a multi-zone phenomenological combustion model for RCCI dual-fuel engines.

Among the recent articles focusing on n-heptane as the chemical surrogate for the diesel fuel, Zhang et al. (W. Zhang et al., 2019) presented a diesel/natural gas dual fuel mechanism (79 species, 224 reactions), employing peak concentration analysis (PCA) and rate of production (ROP) methods to simplify the GRI-mech 3.0 natural gas mechanism, and then combined it with the 95/5 vv mechanism of diesel combustion (represented by n-heptane and aromatic combinations). They validated the reduced mechanism through chemical kinetics calculations and CFD simulations. Although it accurately predicts combustion characteristics and pollutant emissions, the scope is limited to medium-load conditions. Huang et al. (Huang et al., 2019) developed a reduced mechanism (143 species, 746 reactions) based on detailed mechanisms for n-heptane, n-butylbenzene, NG, and polycyclic aromatic hydrocarbons (PAH) using the methods of DRGEP, ROP, and sensitivity analysis. They validated their mechanism against various parameters such as ignition delay and laminar flame speed in the context of HCCI applications, demonstrating its accuracy at varying rates of natural gas substitution. However, the complexity of the mechanism might pose challenges for practical implementation in simulations. Schuh et al. (Schuh and Winter, 2020) proposed a dual fuel combustion mechanism (75 species, 344 reactions), specifically focusing on the ignition and combustion of methane/propane/n-heptane fuel blends in high-pressure environments. They analyzed and updated the Arrhenius parameters to extend the mechanism's application range and included the San Diego nitrogen sub-mechanism to allow for consideration of NOx formation.

As discussed, NG/diesel is one of the most promising fueling strategies for RCCI combustion. Although some mechanisms exist to simulate combustion with these fuels, the present work aims to introduce a compact mechanism designed for high-speed simulations, tailored specifically to the operating conditions of these engines. The mechanism is finally validated through simulations of some RCCI engine cases with both 3-D CFD and multi-zone methods and also fundamental ignition delay time (IDT) and laminar burning velocity (LBV) test data.

2. MATERIALS AND METHODS

The current work targets to develop a chemical kinetics mechanism capable of simulating combustion processes in engines employing multi-fuel low temperature combustion (LTC) strategies, such as RCCI. The targeted fuels include diesel fuel, chosen for its high reactivity, and low reactivity fuels can be a blend of natural gas and hydrogen (H_2). It is assumed that n-heptane (C_7H_{16}) serves as the surrogate for diesel fuel, as demonstrated in numerous scientific investigations on light diesel fuel combustion in engines. Additionally, methane (CH_4) and ethane (C_2H_6) hydrocarbons are incorporated into the mechanism to simulate natural gas reactions.

The mechanism is intended for use in 3-D Computational Fluid Dynamics (CFD) simulations and fast multi-zone models, necessitating a limited number of species and reactions to maintain computational affordability. Hence, skeletal and reduced base mechanisms are employed to construct a multi-fuel mechanism.

In the simulation of combustion processes like RCCI, the auto-ignition of the high reactivity fuel (e.g., diesel) is pivotal in determining the onset of combustion. Unlike applications such as furnace burners, this process begins at relatively high pressures (above 20 bar) and low temperatures (below 900 K) in engine environments. Therefore, selecting a proper set of reactions that accurately predict the ignition of n-heptane under such conditions is crucial. To address this, the skeletal n-heptane mechanism developed by Chang et al. (Chang et al., 2022) is chosen to provide the sub-mechanisms pertinent to n-heptane combustion. This skeletal mechanism is based on the detailed n-heptane mechanism developed by Zhang et al. (K. Zhang et al., 2016), which has been validated against experimental IDT and LBV, establishing its efficacy for n-heptane combustion simulation under engine-like conditions.

To consider reactions related to natural gas (NG) combustion, the GRI 3.0 mechanism (Smith et al., 2000), widely acknowledged as a comprehensive model for NG combustion, is merged with the n-heptane mechanism. To enable the mechanism to predict nitrogen oxide emissions, some corresponding species and reactions are added from the mechanism of Wang et al. (B. Wang et al., 2023).

After merging base mechanisms and adding needed species and reactions, to result a compact mechanism, the DRGEP method with sensitivity analysis is employed to reduce the mechanism. In this, operation the IDT for n-heptane and methane/n-heptane blend mixtures and LBV for methane, methane/H2 and H2 cases are considered as the base cases.

The resulting mechanism comprises 60 species and 372 reactions, which makes it a really compact one comparing to other existing NG/diesel mechanisms.

As previously mentioned, it is crucial for a mechanism intended for RCCI engine simulations to accurately capture the low-temperature auto-ignition of the highly reactive fuel. In this work, the ignition delay resulting from the n-heptane fuel mechanism is compared to the data presented in the study by Zhang et al. (K. Zhang et al., 2016), and adjustments are made to improve agreement with experimental data, particularly for elevated pressures (20 bar) and low temperatures. In RCCI engines, the auto-ignition initiates in mixtures with lower temperatures than 1000 K. Therefore, the combustion IDT should be predicted well by mechanism in this low temperature conditions.

This tuning process involves modifying certain reactions to enhance the mechanism's predictive capability for experimental data.

All merging, reduction, simulations, and optimization processes are conducted using Converge CFD 3.1 software. In the tuning process, the most sensitive reactions under the specified conditions (n-heptane fuel, high pressure, low temperature) are first identified. The sensitivity to these reactions is illustrated in Fig. 1.

In the subsequent stage, the 20 most sensitive reactions are selected, and their pre-exponential factors are optimized using the NLOPT optimization algorithm, which is integrated into the chemistry module of the Converge software. This optimization process aims to align the simulated IDT with the experimental data reported in (K. Zhang et al., 2016).

To assess the effectiveness of the tuning process, a comparison between the IDT resulting from the initial merged mechanism (prior to tuning) and the tuned mechanism against experimental data is presented in Fig. 2. Accurate modeling of the start of combustion in RCCI engines hinges on the mechanism's ability to predict first-stage ignition delay times, which significantly impacts the low-temperature heat release during engine combustion.

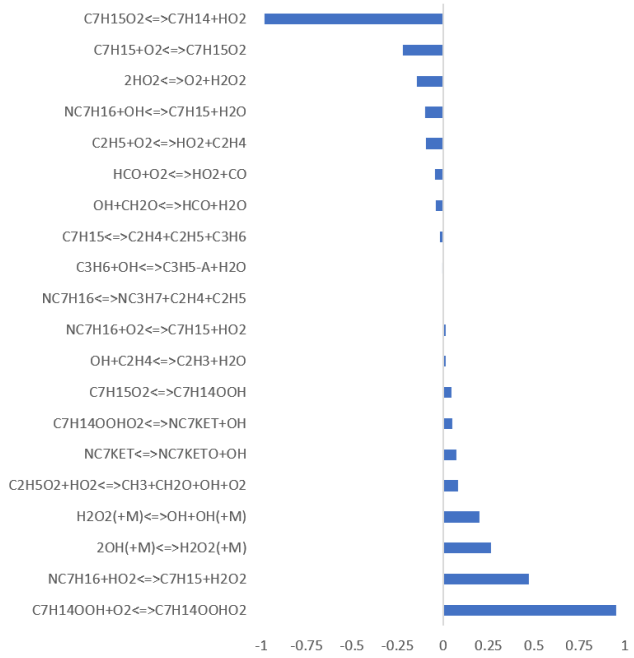

Fig. 1. Sensitivity analyzes for IDTs to identify the most sensitive reactions

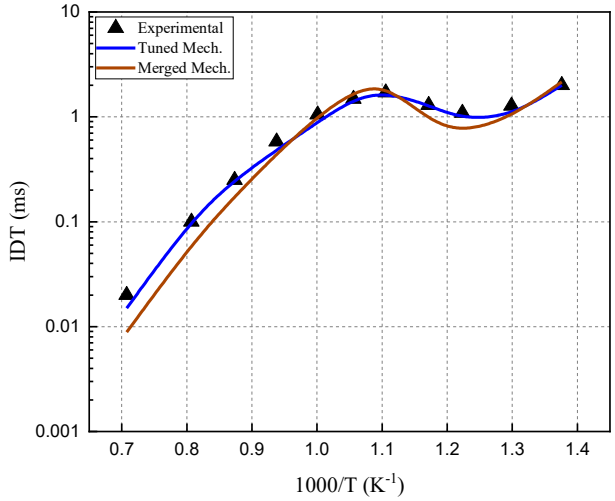

Fig. 2. Comparison of IDT for tuned and merged mechanism with experimental data from Zhang et al. (K. Zhang et al., 2016)

Figure 2 illustrates that following tuning, the mechanism demonstrates improved precision in predicting IDT for n-heptane fuel, particularly within the low-temperature zone. This enhancement renders the mechanism more suitable for simulating engines employing low temperature combustion (LTC) strategies.

3. VALIDATION OF THE NEW MECHANISM

In this section, the performance of the new mechanism is evaluated through simulations compared against available experimental test data. Initially, the IDT and LBV produced by the mechanism are scrutinized against experimental data. Subsequently, the applicability of the mechanism is explored in simulating RCCI and dual-fuel engines with a 3-D CFD software and also a multi-zone code.

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3.1 IDT and LBV simulations

In the context of applying a mechanism for simulation in CI engines, precise prediction of ignition onset time is paramount. Therefore, investigating the IDT resulting from the mechanism across various scenarios is crucial. As the high reactivity fuel in this work is n-heptane and its auto-ignition starts the combustion process, the ability of the mechanism to predict the IDT for n-heptane mixtures is studied in this part.

Figure 3 shows the comparison of IDT values predicted from the new mechanism and mechanisms from Hocket (Hockett et al., 2016) and Rahimi (Rahimi et al., 2010), which are two mechanisms that are widely used for simulation of dual fuel and RCCI combustion in NG/Diesel fueled engines, with experiments of Zhang for n-heptane fuel (K. Zhang et al., 2016). The initial pressure in the tests and simulations is 20 bar and 38 bar, for Fig. 3 (a) and (b) respectively. Hocket mechanism has 150 species and 872 reactions and Rahimi mechanism has 76 species and 483 reactions. The proposed mechanism is seen to give better predictions than the two other mechanisms, although it has less number of species and reactions.

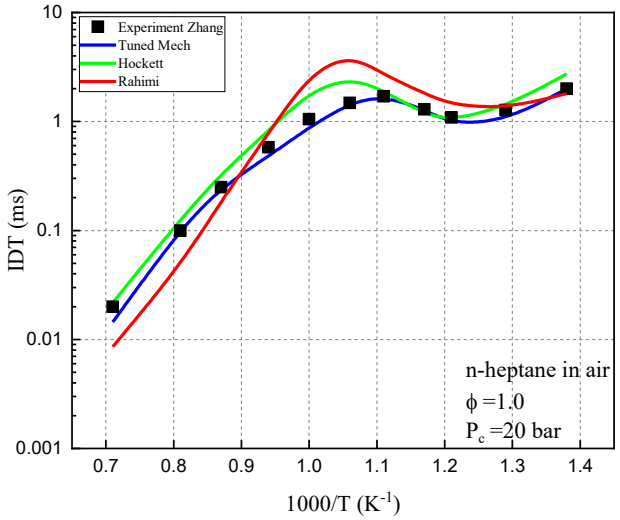
As stated earlier, in the target combustion strategies (RCCI and dual fuel), the auto-ignition process starts from regions with high concentration of the fuel with high reactivity and then the flame propagates into the mixture containing the low reactivity fuel (or fuel blend). Therefore, in the following, the LBV in the mixtures containing target low reactivity fuels, i.e. NG and hydrogen is investigated.

As the first evaluation of flame propagation properties, a 1-D simulation of laminar flame speed in natural gas (NG) was conducted using Converge CFD software. The test case utilized experimental data as reported in (Rozenchan et al., 2002). In this scenario, the initial temperature (pre-burning) was set at 298 K, and initial pressures of 1 atm, 2 atm, and 5 atm were investigated. Figure 4 illustrates the comparison between simulated LBV values and the experimental data reported for different pressures in fuel equivalence ratio (φ) ranged from 0.6 to 1.4. The results indicate that the new mechanism reliably predicts flame propagation within NG mixtures across the investigated range.

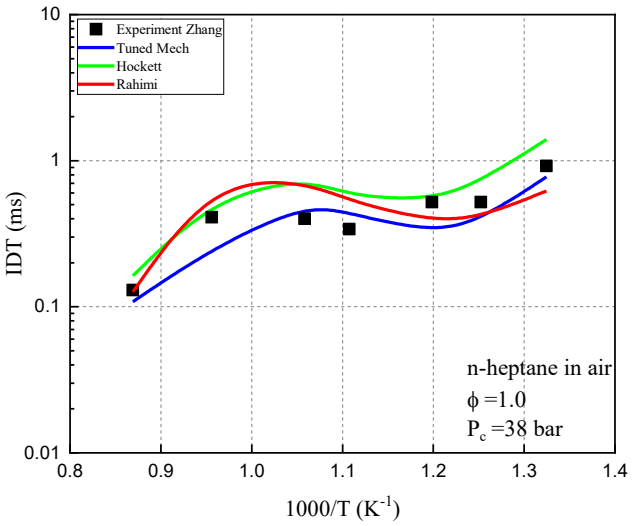
The mechanism is supposed to have the potential to be used for the cases of hydrogen addition to the NG fuel. Graphs of Figure 5 shows the result of LBV simulation for H2/NG fuel blends in both air and O2/He oxidizer environment. Comparison to experimental cases reported by Donohoe et al. (Donohoe et al., 2014) shows that the new mechanism has a good ability to predict flame propagation in H2/NG blend mixtures, as well as mixtures of air and NG. Specially, it is seen that the simulations have a very good accuracy to predict the results close to experimental data, for lower equivalence ratios than 1 in the low reactivity mixture, which is the case that usually happens in the target dual fuel and RCCI engines.

3.2 Simulation of RCCI NG/diesel fueled engines

To verify the mechanism ability in simulation of combustion in NG/diesel fueled engines, two marine engines with RCCI combustion mode are selected to be both experimentally and numerically investigated. First one is the 6L20CRDF research engine, a variant of the Wärtsilä 20 platform, featuring a 6-cylinder inline dual fuel (DF) configuration (Kakoee et al., 2023). The second investigated marine engine is a Wärtsilä single-cylinder research engine (SCRE), which adheres to the DF variant of Wärtsilä's W31 engine platform (Åstrand, 2016). Key specifications of both test engines are outlined in Table 1.



(a)



(b)

Fig. 3. Comparison of IDT for the new mechanism with two other mechanisms (Hockett (Hockett et al., 2016) and Rahimi (Rahimi et al., 2010)) and also experimental data from Zhang et al. (K. Zhang et al., 2016), for (a) pressure of 20 bar and (b) pressure of 38 bar

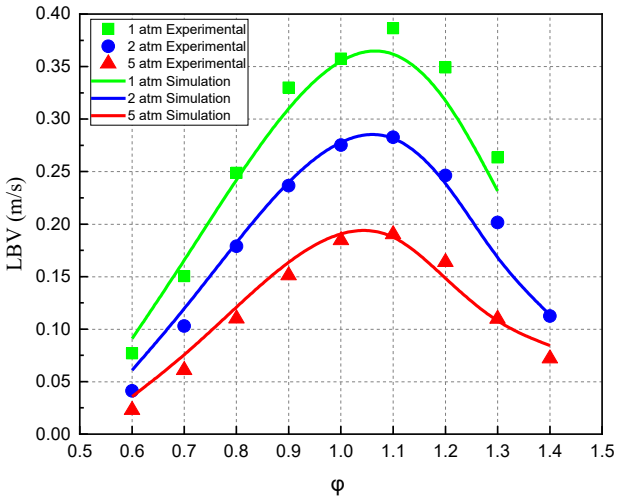


Fig. 4. LBV for NG mixtures in different pressures, comparison of simulations (lines with small marks) with experimental data (marks) from Rozenchan et al. (Rozenchan et al., 2002)

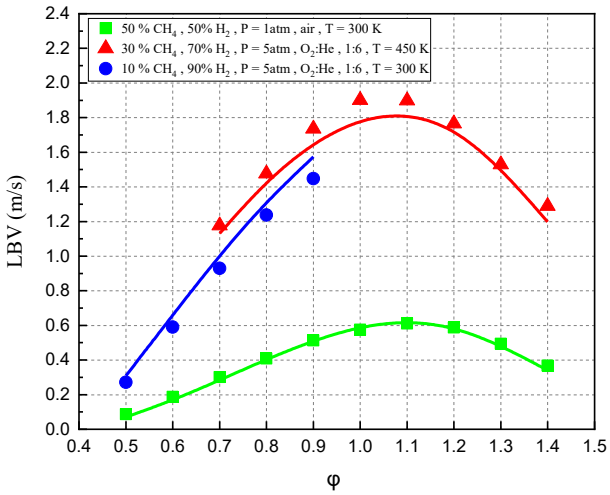


Fig. 5. LBV for NG/H2 mixtures in different pressures and blend ratios comparison of simulations (lines with small marks) with experimental data (marks) (Donohoe et al., 2014)

3.4 3-D CFD simulation

In this part, 3-D CFD simulation of a closed cycle (IVC to EVO) for Wärtsilä W20 engine with RCCI combustion is performed using Converge CFD v3.1 software. The SAGE solver, specializing in transient chemical kinetics, was used in transient mode to compute species mass fractions at each time step before solving the transport equation with the PISO technique. Diesel fuel properties were represented by the "DIESEL2" surrogate from the CONVERGE library for spray and mixing modeling. Liquid injection was modeled using the Blob injection sub-model, with parcel diameter set to the nozzle hole size. Diesel spray was simulated with the KH-RT model considering high injection pressure. Heat transfer was modeled using the Standard Wall Function, while turbulence was captured via the RNG k-ε model. Adaptive mesh refinement was used for a base grid size of 0.002 m.

Computational runs are conducted to evaluate RCCI operation of the engine using diesel and NG fuels under mid-load conditions. For the simulated case, the energy share of diesel and NG fuels were 7% and 93% respectively. In this scenario, diesel fuel injection has commenced about 70° before piston TDC, allowing for partial mixing of diesel fuel with the in-cylinder mixture, facilitating RCCI combustion mode.

Figure 6 illustrates a comparison between simulated and measured in-cylinder pressure and heat release rate (HRR) to assess the performance of the mechanism in simulating diesel/NG combustion. Normalized values are presented in the figure, relative to their maximum values. The depicted results demonstrate a high level of agreement between simulation and measurement. Both the pressure trace and heat release processes are simulated with acceptable accuracy. Important operating parameters such as SOC, maximum pressure and maximum HRR are seen to be predicted with a good accuracy. The results prove the effectiveness of the new mechanism for simulating combustion processes in mixtures containing diesel fuel and NG under internal combustion engine conditions.

Table 1: Specification of the Wärtsilä test engines

Engine model	**Wärtsilä W20**	**Wärtsilä W31**
Displacement	8.8 liter	32.45 liter
Stroke/Bore	1.4	1.39
Test Speed	1000 rpm	720 rpm
Air System	Two-stage turbocharged (in series)	External air compressor with air temperature and pressure control (up to 10 bar)
High reactivity fuel system	Common rail	Common rail 2.0 with twin needle injector; and multi-injection capability
Low reactivity fuel system	Low-pressure; multi-point, upstream of the intake valve	Low-pressure, multi-point, upstream of the intake valves
Valve train	4 valves per cylinder, fully variable hydraulic valve train	four valves with swirl + tumble ports; variable intake valve closure (VIC); fixed exhaust valve opening (EVO)

3.5 Quasi-dimensional simulation

In this section, simulations are conducted using the UVATZ code, a multizone model developed at Vaasa University specifically designed to model combustion in RCCI engines (Vasudev, Cafari, et al., 2022). UVATZ simulates low-temperature combustion concepts driven by chemical kinetics and in the present study, is parameterized for natural gas and diesel RCCI combustion. The model accounts for fuel and thermal stratification, in-cylinder turbulence, IVC temperature, and residual gas composition. It consists of 12 zones, two disc-shaped for the cylinder head and piston boundary layers, and 10 annular zones, with the outermost in contact with the liner, capturing bulk inhomogeneity. Heat and mass flows are modeled through gradient-based transport.

HRF stratification is simplified, with mass linearly distributed across the zones, and evaporation enthalpy proportional to HRF mass.

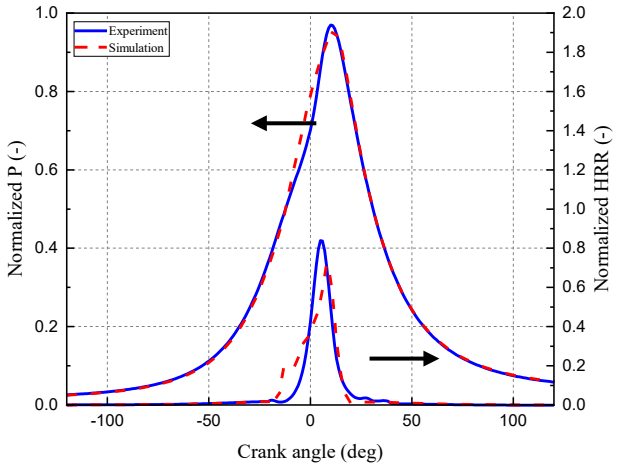


Fig. 6. Comparison of in-cylinder pressure and HRR (normalized values) between experiments and simulation for an NG/diesel RCCI engine in CFD simulation

The simulated engine under study is a Wärtsilä single-cylinder research engine (SCRE), which adheres to the dual fuel (DF) variant of Wärtsilä's W31 engine platform (Åstrand, 2016).

In the tests conducted for this segment, the load is about 25% of the full load conditions. Liquified natural gas (LNG) with a methane number of 80 serves as the low reactivity fuel, while light fuel oil (LFO) acts as the high reactivity fuel. The start of injection of LFO occurs 65° before top dead center (TDC) to ensure the onset of RCCI combustion. Notably, 70% of the total fuel energy is attributed to NG, while the remaining 30% comes from LFO.

The 12-zone configuration of the UVATZ model, which is employed in the present work, has the ability to represent the subtleties of fuel and thermal stratification, in-cylinder turbulence, intake valve closing (IVC) temperature, and the composition of residual burned gas. These zones interact with one another through the transfer of heat, mass, and work, making them dynamic entities in the simulation world. The model also accounts for heat loss to the walls, which is modeled using a specific correlation (Kakoee et al., 2023).

For simulations, n-heptane serves as a surrogate for LFO, whereas a mixture of methane and ethane is employed to represent NG. A 13-zone model is utilized for quasi-dimensional modeling of the RCCI combustion process.

Figure 7 presents a comparison between measured and simulated in-cylinder pressure curves and heat release rate. The simulation process, executed on a PC with an i7-13700H processor, required 219 seconds for a full-cycle simulation to converge. For the presented engine test case, it took 4 cycles for the model to converge. It is evident that certain parameters, like SOC and peak pressure, have been accurately predicted. This comparison highlights the mechanism's suitability for integration into multi-zone model codes to simulate the RCCI combustion process.

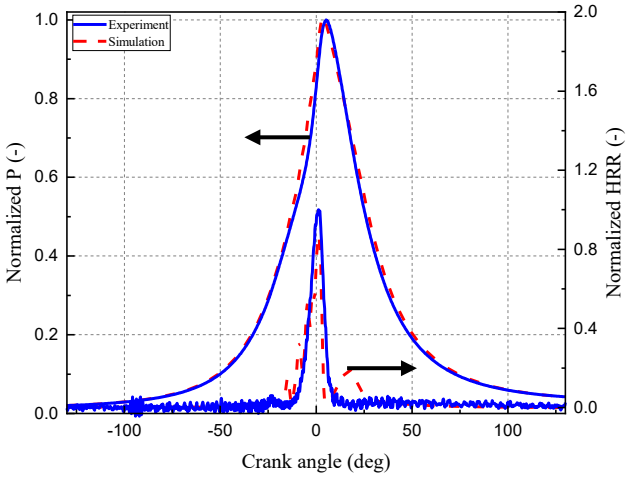


Fig. 7. Comparison of in-cylinder pressure for experiments and simulation for an NG/diesel RCCI engine with MZM code

4. CONCLUSION

A reduced chemical kinetics mechanism for NG, H_2 / n-heptane blends was proposed in this study. This mechanism contained 60 species and 372 reactions, making it cost-effective for simulation of combustion engine cases. The mechanism was formed based on merging existing mechanisms for n-heptane, and NG. The mechanism was tuned for better resolving n-heptane auto-ignition in low temperatures and elevated pressures. The mechanism's accuracy was initially assessed using fundamental Induction Delay Time (IDT) and Laminar Burning Velocity (LBV) experimental data from the literature for the blended target fuels. It was demonstrated that 0-D simulations employing the new mechanism could accurately predict the IDT for n-heptane fuel mixtures with acceptable precision, better than some of other widely used mechanisms for NG/diesel fueled engines. Furthermore, conducted 1-D simulations substantiated the mechanism's capability to predict LBV in mixtures of target low reactivity fuels, considering mixtures with NG and NG/H_2 blends. After verification with data from fundamental tests, 3-D CFD simulation utilizing this new mechanism were validated with real engine test data, for NG/diesel cases. Good agreement between test results and simulations demonstrates the mechanism's suitability for simulating engines operating in multi-fuel modes such as RCCI and dual fuel, with diesel as the high reactivity fuel and a blend of NG and H2 as the low reactivity fuel.

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