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NUMERICAL SIMULATION OF A PREMIXED DUAL-FUEL COMBUSTION IN A CONSTANT VOLUME COMBUSTION CHAMBER

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ABSTRACT

The dual-fuel (DF) combustion concept is one of the promising strategies for modern automotive and marine engines to achieve lower emission levels. A premixed DF engine operates by having a pilot diesel injection to ignite the lean premixed natural gas in the engine. Experimental studies on premixed DF combustion with micro pilot diesel fuel are limited. Hence, the underlying mechanism are still not well-understood. In this study, a three dimensional (3D) computational fluid dynamic (CFD) study is performed using the Simcenter Star-CCM+ software to investigate the ignition characteristics of the premixed DF combustion. Large eddy simulation (LES) is used for the turbulence modelling in the current work. The numerical simulation is carried out by modelling the injection of the pilot diesel fuel into a constant volume bomb with a premixed methane-air mixture. The adaptive mesh refinement (AMR) is implemented in order to increase the computational efficiency. The minimum cell size is set to 0.25 mm. N-dodecane fuel is used as a pilot diesel surrogate fuel. Two reduced n-dodecane chemical mechanisms, i.e. Yao53 and Lapointe63, are being tested. Model validation is carried out by comparing the liquid penetration length (LPL) of the inert diesel spray to the measured data. The predicted ignition delay time (IDT) in the pure diesel case and the DF case are also validated against the available experimental data. Both mechanisms are able to capture the ignition process in the pure diesel case with reasonable accuracy, with the Lapointe63 mechanism having relatively better performance. However, only Lapointe63 is able to capture the ignition process in the DF case. The discrepancies observed in the simulation results may be attributed to the mechanism itself and the assumption that premixed methane/air is homogeneously mixed.

Keywords: Premixed dual-fuel, Methane gas, Pilot diesel injection, Large eddy simulation, Constant volume combustion chamber

INTRODUCTION

The dual-fuel (DF) combustion concept constitutes a promising strategy for modern gas engines, especially in the maritime industry, to achieve simultaneously low emissions of unburned hydrocarbons (UHC) as well as nitrogen and sulfur oxides (NO_x

and SO_x). These modern gas engines commonly use natural gas as a main fuel. However, the low reactivity of the lean premixed charges renders reliable ignition difficult. Therefore, a micro-pilot injection of a highly reactive liquid fuel is used to ensure successful combustion initiation in DF engines. As natural gas consists mainly of methane gas, methane is generally treated as the representative of the natural gas. N-dodecane or n-heptane are commonly selected as the diesel surrogate. It has been observed in the engine experiments that the ignition of the diesel spray is retarded if the ambient air contains methane [1; 2]. This is confirmed by numerous experimental studies which were carried out in fundamental reactors, such as shock tube (ST) [3; 4].

It is worth mentioning that the in-cylinder flow varies from one engine to another due to the different engine configurations. Meanwhile, the injection characteristics are also not standardized, which may result in varying air/fuel mixing as well. These collectively make direct comparison of the results from different DF engine data difficult. To better understand the ignition characteristics of the DF combustion without the complex in-cylinder flow, experimental studies can be carried out in a constant volume vessel with controlled ambient pressure and temperature conditions which resemble those of direct injection diesel engines. Recently, Yang et al. [5] have successfully demonstrated the feasibility of performing the premixed DF combustion in a constant volume combustion chamber. The experiment involves injecting a pilot-diesel fuel into a premixed methane/air mixture. They have also shown that diesel spray ignition is delayed when methane fuel is present.

To gain a better understanding of the ignition process in a premixed DF configuration, numerical simulations in a constant volume chamber are carried out. Wei et al. [6] and Zhao et al. [7] performed large eddy simulation of n-heptane spray in a premixed methane/air environment under the Spray H condition from ECN [8]. In addition, Kahila et al. [9] and Tekgul et al. [10] have performed numerical simulations to investigate the DF ignition process of n-dodecane spray injection into a methane-air mixture. Their simulations were carried out in a constant volume chamber under the Spray A condition from ECN [8]. In all of the aforementioned numerical studies in constant volume com-

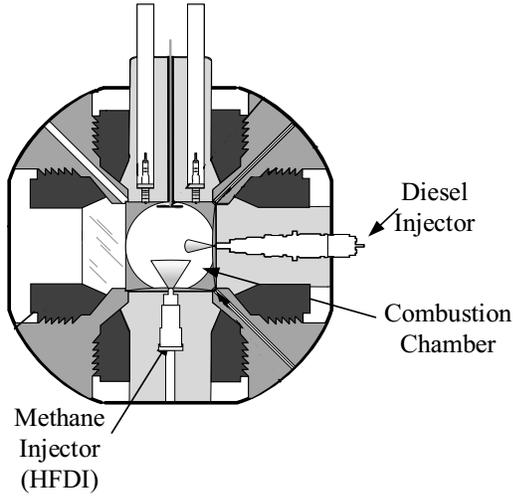


Figure 1. Schematic cross-section of the spray and combustion vessel for DF experiment. Figure adopted from Refs.[5; 11].

combustion chamber, presence of methane is shown to increase the ignition delay time (IDT) of the injected diesel spray. However, none of them have validated their DF combustion results against the experimental data.

Setting against this background, the present study aims to investigate the performance of different reduced n-dodecane mechanisms in premixed DF combustion by validating the simulated results against the measurements from the experimental study conducted separately by Yang et al.[5]. This is achieved by performing both 0-D homogeneous reactor calculations and three-dimensional (3-D) computational fluid dynamic (CFD) spray modeling.

CASE DESCRIPTIONS

Numerical simulations in the present study are based on the experimental study carried out by Yang et al. [5]. Full details of the experimental setup and procedure to achieve diesel/methane DF combustion process in a constant volume combustion chamber are available in Refs. [5; 11]. Only a brief description of the experimental setup is mentioned here for completeness.

Figure 1 shows the schematic cross-section of the constant volume combustion vessel for DF experiment [5; 11]. The experiment is carried out in an optically accessible 1.1 L cubic-shaped combustion chamber. Two injectors are installed onto the system, where one is for the pilot diesel injection and another for the methane gas injection. An 8-hole injector with hole diameters of 0.169 mm and an included angle of 150° is used as the pilot diesel injector. The injection pressure and electric injection duration (EID) are set to 1000 bar and 0.25 ms, respectively. A total injected mass of 1.7 mg is obtained during the pilot diesel injection. The diesel fuel used in the experiment has a fuel density of 784 kg/m^3 and cetane number of 85. On the other hand, methane gas is injected from a single-hole injector with hole diameter of 0.5 mm and injection pressure of 200 bar.

To replicate the engine thermodynamics and the premixed

Table 1. Ambient composition and operating conditions for diesel and dual-fuel cases.

	Case 1 (Inert, Diesel)	Case 2 (Diesel)	Case 3 (Dual-fuel)
T_{am} [K]	453	750	750
ρ_{am} [kg/m^3]	13	13	13
Composition [% mol]			
Nitrogen, N_2	100	74.6	70.0
Oxygen, O_2	0	15.9	15.9
Methane, CH_4	0	0	4.6
ϕ_{CH_4} [-]	-	0	0.58

conditions representative of a DF engine inside a constant volume combustion chamber, the following steps are taken in experimental study by Yang et al. [5]: the standard pre-burn process is conducted using a lean mixture of acetylene, hydrogen, oxygen, and nitrogen to generate a high-temperature mixture with the desired oxygen concentration. In the pure diesel spray combustion case, pilot diesel fuel is injected once the post-burn products cool down to the desired ambient conditions. However, in the DF combustion case, methane gas is injected into the chamber and allowed to mix prior to the pilot diesel fuel injection. A minimum mixing duration of 50 ms is suggested by Yang et al. [5] to be sufficient for the injected methane to mix with the ambient gas inside the combustion chamber to produce a homogeneous methane/air mixture.

It is important to note that, the methane injection process and mixing process are not considered in our numerical simulations to avoid the additional computational cost it may incur. Therefore, methane gas is assumed to be mixed homogeneously with the ambient mixture to form a premixed methane/air mixture prior to the pilot diesel fuel injection in the DF case.

The ambient mixture composition and operating conditions for the diesel and DF cases are shown in Table 1. Case 1 is an inert diesel case, which is carried out in a pure N_2 mixture with an ambient temperature (T_{am}) of 453 K. Case 2 and 3 are reacting diesel and DF cases, respectively, at an O_2 level of 15.9%. Methane is present in the ambient mixture of Case 3, where the methane equivalence ratio (ϕ_{CH_4}) is equal to 0.58. In all cases, the ambient density (ρ_{am}) is set to 13 kg/m^3 .

CFD MODEL DESCRIPTIONS

The simulation works in the present study are carried out using the CFD software Siemens Star-CCM+ version 15.06.008-R8. The gas-phase flow and combustion processes are modeled in an Eulerian framework. Meanwhile, the motion of the liquid-phase is modeled in the Lagrangian framework.

Spray and injector model

The 8-holed diesel injector is located at $l_{\text{disp}} = 11 \text{ mm}$ and $W = 51.6 \text{ mm}$ from the wall boundaries, as depicted in Figure 3.

The injector holes are assumed to be equally distributed along a circle with a radius (r) of 1 mm. The injector is modeled as a solid cone injector with a liquid spray angle of 20° .

The Lagrangian Particle Tracking (LPT) method is used to model the discrete dispersed liquid phase injected from the injector. Droplets of similar quantities are clumped together namely a parcel, to drastically reduce the computational cost. The primary spray breakup is considered by sampling computational parcels from the Rosin-Rammler size distribution, where the maximum droplet diameter is specified as 50% of the diameter of a single hole (i.e. 0.169 mm). The reference diameter is specified as $\exp(-1)$, which is $\sim 33\%$ of the maximum droplet diameter, while the minimum droplet size is set as $1\ \mu\text{m}$. The secondary spray breakup is modeled by the Reitz-Diwakar breakup model [12].

Turbulence and combustion model

In the present study, the gas flow field is solved for the filtered Navier-Stokes equations under the Eulerian framework. The sub-grid scale is modeled by the dynamic Smagorinsky model [13]. The Laminar flame concept (LFC) model, which is also known as well-stirred reactor (WSR) model, has been chosen as the combustion model. The model assumes that the mixture is homogeneous in each computational cell, hence no turbulence-chemistry interactions is considered in this model. This model has been used by other spray combustion studies [14; 15].

Computational domain and numerical scheme

The computational domain is a constant volume cubic chamber with side lengths of 103.2 mm, which corresponds to the 1.1 L combustion vessel in experimental study [5]. The ambient mixture composition, pressure, and temperature from Table 1 are initiated as uniform field while the velocity field is set to zero. All boundaries are set as no-slip wall with Neumann boundary condition for the ambient mixture composition and pressure. A constant wall temperature of 453 K is assumed for walls.

The numerical simulations use adaptive mesh refinement (AMR) with a base mesh size of 2 mm and a minimum mesh size of 0.25 mm. A fixed cylindrical refinement zone with 0.25 mm mesh size is created in the vicinity of the liquid diesel spray region (cf. Figure 3) to capture the high-velocity liquid spray. Any spray exiting the refinement zone will cause the mesh around it to be dynamically refined via AMR method. At the same time, an adaptive time-stepping method is also implemented in all of the numerical cases where the minimum time-step and maximum Courant number are set to 25 ns and 0.3, respectively. The spatial and temporal terms are discretized by second-order schemes.

Chemical kinetic model

In this study, n-dodecane ($\text{C}_{12}\text{H}_{26}$) fuel is assumed to be the surrogate for the diesel fuel used in the experiment [5], as their cetane number as close to one another. Two reduced n-dodecane mechanisms are considered in the present study: the 53-species mechanism by Yao et al. [16] and the 63-species mechanism by Lapointe et al. [17]. Detailed description of each mechanism can

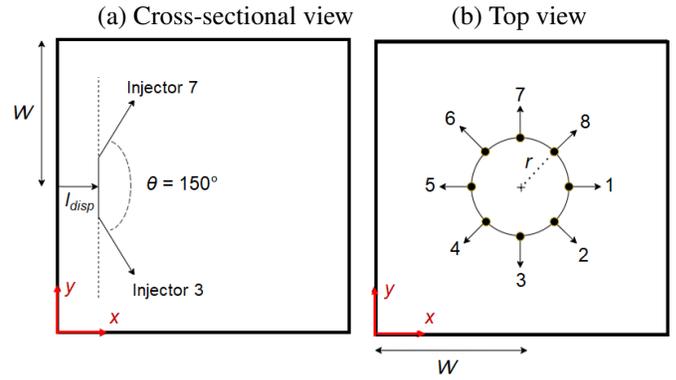


Figure 2. Illustration of the combustion chamber geometry and the location of diesel injector nozzle holes.

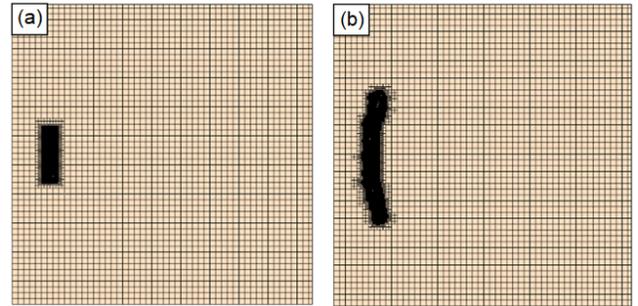


Figure 3. Cross sectional view of the mesh constructed (a) before running and (b) after running the simulation.

be referred to their respective publication. For brevity, the mechanism by Yao and Lapointe are henceforth known as Yao53 and Lapointe63, respectively. Yao53 has shown a good performance in the homogeneous n-dodecane-air ignition problems [16] and in the n-dodecane spray combustion context [9; 10; 14; 18]. The performance of Lapointe63 can be seen from ECN 7 proceedings [8]. It is worth mentioning that both mechanisms contain the relevant subset of reactions to describe the methane ignition chemistry. In order to evaluate the performance of these mechanisms to model the methane oxidation in lean conditions, IDT results from 0-D homogeneous reactor model are performed and compared against the experimental data from Davidson and Hanson [19]. The reactor model is assumed to be a closed, homogeneous, constant volume and adiabatic. The IDT is defined as the time where the maximum rate of temperature rise in the system.

Figure 4 illustrates the IDT of methane/oxygen mixture at fuel-lean mixture of $\phi_{\text{CH}_4} = 0.4$ and $P_{\text{am}} = 48\ \text{atm}$. Both Yao53 and Lapointe63 show qualitatively good agreement with the measurements [19]. In addition, laminar flame speed (LFS) is also computed to complement the IDT results. Figure 5 shows the predictions of the laminar flame speeds in methane/air mixtures at ambient pressures of 1 atm and 10 atm. The initial unburned fuel temperature is set to 300 K. Both mechanisms show comparable LFS prediction to the measurement by Rozenchan et al. [20], with Lapointe63 having relatively better performance.

Overall, both mechanisms show good correlation between the

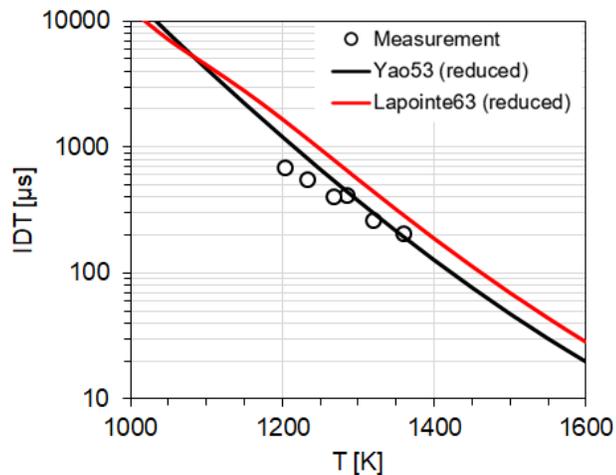


Figure 4. Ignition delay times (IDT) of methane/oxygen under fuel-lean condition (3.8% CH₄+19.2% O₂ in Argon, $\phi_{\text{CH}_4} = 0.4$) at $P_{\text{am}} = 48$ atm. Measurements from Ref. [19].

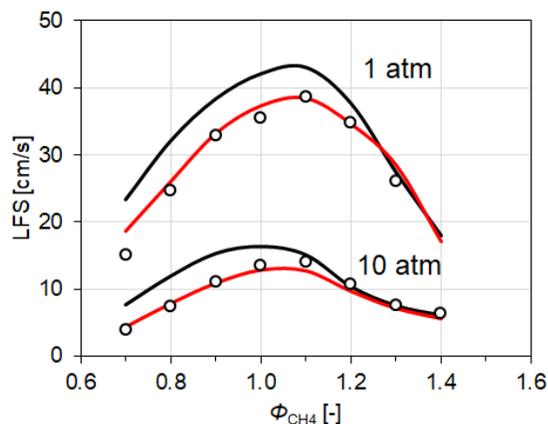


Figure 5. Laminar flame speed (LFS) of methane/air mixture at P_{am} of 1 and 10 atm. Measurements from Ref. [20]. Please refer to Figure 4 for the legends.

experimental and simulated IDT and LFS for methane/air mixtures in 0-D studies. Hence, both mechanisms are tested next in 3-D CFD simulations.

RESULTS AND DISCUSSION

Inert diesel spray

Before performing reacting spray simulations, the computational setup is first validated by comparing the liquid penetration length (LPL) with the measured data. LPL is defined here as the maximum axial distance encompassing 95% of the liquid fuel mass. Figure 6 shows the temporal evolution of the liquid penetration length of inert sprays from the experiments and numerical model. The predicted LPL is depicted to correspond reasonably well with the measured LPL data, which indicates that the numerical setup is able to capture the spray characteristics. The numerical setup is next used to simulate the reacting spray cases.

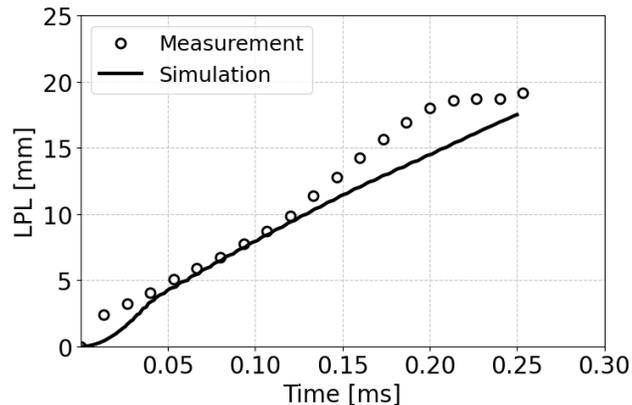


Figure 6. Liquid penetration length (LPL) of the inert diesel spray simulation. Measurements from Ref. [5; 11]

Reacting diesel and dual-fuel spray combustion

Numerical simulations of two reacting spray configurations are carried out, i.e. the diesel and DF case (see cases 2 and 3 in Table 1). The Yao53 and Lapointe63 mechanisms are utilized to simulate both the diesel and DF cases to evaluate their performance in the 3-D CFD simulations. The IDT for the 3-D CFD simulations is defined as the time where the maximum rate of temperature rise in the system, which is in accordance to the recommendation by ECN [8]. The IDT in the experiment is defined as the time between the start of diesel injector hydraulic opening and the first frame that diesel auto-ignition is identified in Schlieren images [5].

Figure 7 shows the temporal evolution of T_{max} for the diesel and DF cases using the Yao53 and Lapointe63 mechanisms. For the diesel cases, Yao53 and Lapointe63 predicts IDT of 2.45 ms and 3.08 ms, respectively (cf. Figure 7). Comparison to the experimental diesel IDT of 1.6 ms yields a relative difference of 93% and 53% for Yao53 and Lapointe63, respectively. The overpredicted IDTs from both Yao53 and Lapointe63 are likely attributed to the difference in defining when ignition occurs.

Based on Figure 7, the DF case IDT for Lapointe63 is depicted to be 4.43 ms, with a relative difference of 29% to the measured data. However, no ignition is captured when using Yao53 in the DF configuration, even when the ρ_{am} is increased to 22.8 kg/m³ (not shown). Meanwhile, it is noteworthy that Yao53 was shown to ignite in another premixed DF configuration [9], but at a higher T_{am} of 900 K with $\rho_{\text{am}} = 22.8$ kg/m³, as well as having longer diesel fuel injection duration (i.e. larger amount of injected fuel). Furthermore, the amount of diesel fuel injected in [9] is higher than that in the present work. In the present work, a micro-pilot injection strategy is considered, where the injected pilot diesel has an equivalent energy contribution lower than 5% of the total energy.

To gain a better understanding of the ignition process in both the diesel and DF configurations, the temporal evolution of the maximum mass fraction (Y_{max}) of CH₂O and OH are shown in Figure 8. Formaldehyde (CH₂O) is a product of the low-temperature ignition which has frequently been mea-

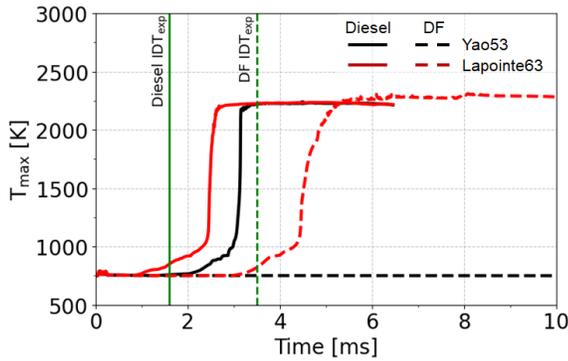


Figure 7. The temporal evolution of maximum temperature (T_{\max}) for diesel and dual-fuel (DF) cases using the Yao53 and Lapointe63 mechanisms.

sured in experiments [21] as a marker of regions where low-temperature (cool-flame) chemistry is underway. Hydroxyl (OH) is selected as a marker of regions where high-temperature chemistry is active, also in accordance with several experimental studies [22; 23]. In the diesel case (Figure 8a), both Yao53 and Lapointe63 show formation of CH_2O and subsequently OH formation, which indicates the occurrence of both low-temperature and high-temperature ignition in the system. However, in the DF case (Figure 8b), Lapointe63 shows both formation of CH_2O and OH, but not for Yao53. The results imply that the low-temperature reaction pathway in Yao53 mechanism may not be able to perform properly in DF spray combustion applications that are at low T_{am} .

Besides examining the ignition processes in the DF configuration, it is also important to examine the combustion process of the premixed methane/air mixture after ignition, the average pressure rise (ΔP_{avg}) in the DF case is examined by comparing the simulation results and the experimental data (cf. Figure 9). Only the results from Lapointe63 are presented in the figure as it is the only mechanism to ignite under the present DF configuration. From the figure, the simulated pressure rise agrees reasonably well with the measurement before 8 ms, but underpredicts from 8 ms onwards. The discrepancies observed in Figure 9 may be caused by the inhomogeneity of the methane/air mixture prior to the pilot diesel fuel injection. Pockets of the ambient mixture that contains less methane may promote the ignition process of the pilot-diesel fuel. Numerous such “pockets” of inhomogeneous local mixture may result in an increase in the number of ignition sites. This may subsequently lead to a faster burning of the premixed methane/air mixture, thus leading to faster pressure rise. Further investigations are necessary to verify this speculation. Overall, Lapointe63 is demonstrated in the present study to be capable of capturing the DF combustion at such a low temperature, density conditions ($T_{\text{am}} = 750 \text{ K}$, $\rho_{\text{am}} = 13 \text{ kg/m}^3$).

CONCLUSION

In this study, a three dimensional (3D) computational fluid dynamic (CFD) study is performed using the Simcenter Star-CCM+ software to investigate the ignition characteristics of the

premixed DF combustion. Large eddy simulation (LES) is used for the turbulence modelling in the current work. The numerical simulation is carried out by modeling the injection of pilot diesel fuel into a constant volume bomb with a premixed methane-air mixture. The adaptive mesh refinement (AMR) is implemented in order to increase the computational efficiency. The minimum cell size is set to 0.25 mm. N-dodecane fuel is used as a pilot diesel surrogate fuel. Two reduced n-dodecane chemical mechanisms (Yao53 and Lapointe63) are being tested. Model validation is carried out by comparing the liquid penetration length (LPL) of the inert diesel spray to the measured data, which shows a good agreement between them. The predicted ignition delay time (IDT) in the pure diesel case and the DF case are also validated against the experimental data. Both mechanisms are able to capture the ignition process in the pure diesel case with reasonable accuracy, with the Lapointe63 mechanism having relatively better performance. However, only Lapointe63 is able to capture the ignition process in the dual-fuel case. It is implied that Yao53 may not be suitable for dual-fuel application that have low ambient temperature ($T_{\text{am}} = 750 \text{ K}$). The discrepancies observed in the predicted IDT and pressure rise curve may be attributed to the mechanism itself and assumption that premixed methane/air is homogeneously mixed.

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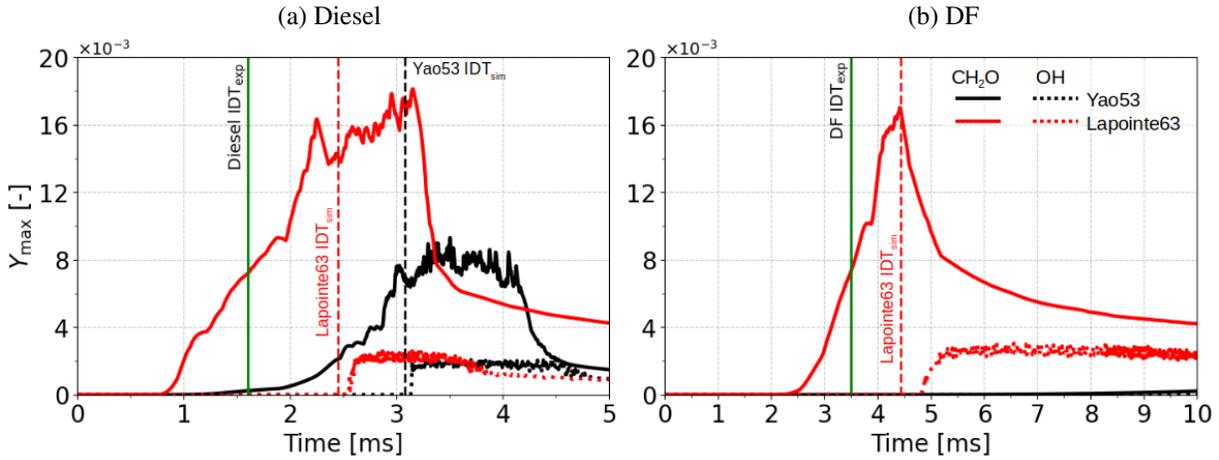


Figure 8. The temporal evolution of maximum mass fraction (Y_{\max}) of CH_2O and OH for (a) diesel and (b) dual-fuel (DF) configurations using Yao53 and Lapointe63 mechanism.

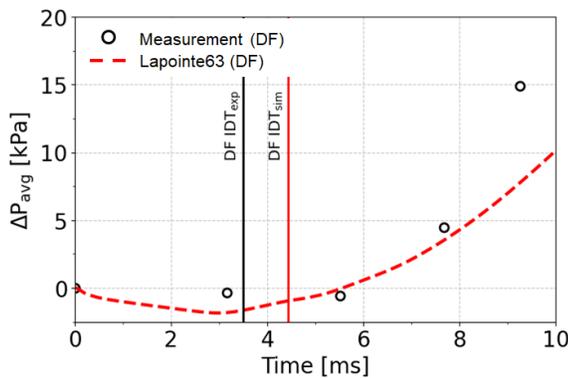


Figure 9. The temporal evolution of average pressure rise (ΔP_{avg}) for the dual-fuel (DF) case using the Lapointe63 mechanism. Measurements from Ref. [5].

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