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Modeling of a Single-Fuel Hydrogen Spark ignition and a Dual-Fuel Diesel-Hydrogen Engines

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Abstract

Most transport vehicles, especially medium and heavy duty trucks, are currently powered by internal combustion engines (ICEs). These engines present a major source of carbon dioxide (CO_2) emissions by burning fossil fuels which have high carbon content. One transitional path towards ultra low CO_2 emissions of ICEs is to redesign them to be able to use alternative fuels like hydrogen fuel that have zero carbon content. Two main types of ICEs are spark ignition engines and CI engines. SI engines burn high octane number fuels so they can run on %100 hydrogen, but CI engines can only use hydrogen in a dual-fuel mode with a primary fuel to start the combustion. In this study, two 0D engine models for a SI hydrogen engine and for a CI dual-fuel diesel-hydrogen engine are developed. Experimental data from these engines is used to calibrate and test the 0D model. The 0D model requires a laminar flame speed calculation. For the laminar flame speed (LFS) calculation, a machine learning neural network based model is used for both of the SI and CI engine models. Small deviations between the simulation and experimental results indicates the laminar flame speed and combustion models are valid. Increasing of the hydrogen energy ratio in dual-fuel mode increases the peak in-cylinder temperature and pressure which results in higher Nitrogen Oxides (NOx) production. The developed 0D engine models provide powerful tools for further engine development, in particular they are useful for the design of model-based combustion control and engine control unit (ECU) calibration.

1 Introduction

Internal combustion engines (ICEs) that are powered by fossil fuels play a crucial role in the transportation sector. The two primary types of ICEs are spark ignition (SI) engines and compression ignition (CI) engines. Almost all ICEs in the transportation sector burn fossil fuels and are a major source of air pollution and carbon emissions production. High carbon content in fossil fuels such as gasoline and diesel produce CO_2 which is a greenhouse gas. One solution to make ICEs produce less CO_2 is to use alternative fuels with low carbon content. This would result in a reduction or even zero carbon production and have been investigated for many engines [1, 2]. Hydrogen is a promising alternative fuel which has zero carbon content. Hydrogen fuel characteristics includes low ignition energy, rapid flame propagation, and high diffusion coefficient. This enables spark-ignition engines to run using %100 hydrogen as fuel [1]. Therefore its deficient for CI engines to run using 100% hydrogen because the compression temperature in these engines is typically insufficient to initiate combustion. CI engines use a second engine to ignite the mixture and they can only use hydrogen in dual-fuel mode [2].

The run of an engine model with hydrogen fuel is used for analyzing the engine's performance under different operating conditions. Different modeling tools have been used to study effects of adding hydrogen into a diesel fuel engines in the literature. Majority of the studies in this field reported that adding hydrogen up to a certain amount could improve engine performance, but it increases NOx emission production as a result of higher combustion temperature. Ghazal [3] simulated dual-fuel diesel-hydrogen engine and reported that adding hydrogen to diesel engine improve engine brake power up to 14%. An et al. [4] used KIVA4 coupled with CHEMKIN to model a hydrogen diesel engine. They concluded that hydrogen addition improves engine performance by increasing the indicated thermal efficiency especially at low loads, but at the same time it

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*Corresponding author: saeidshahpouri@ualberta.ca increases NOx emissions. Masood et al. [5] simulated hydrogen-diesel dual-fuel engine using computational fluid dynamic (CFD) by means of Fluent software. They found out that hydrogen addition to the diesel engine could improve brake thermal efficiency up to %19 and increase NOx production up to 33%. Here, the unique models are developed that could be used for calibration and control purposes.

In this study, a SI hydrogen engine as well as a dual-fuel CI diesel-hydrogen engine are modeled in GT power software as a 0D model. Experimental data from engine experimental setups are used to calibrate and test these models. For the laminar flame speed (LFS) model, a neural network based model is used. After creating the 0D model, experimental in-cylinder pressure trace and NOx emission for engines operating points are used to calibrate the model and to evaluate the model performance.

2 Methodology

A pure hydrogen SI engine and a dual-fuel diesel-hydrogen engine are both modeled in GT power software. GT power is powerful software for 0D and 1D modeling ICEs. A spark-ignition turbulent flame model and dual-fuel combustion model in GT-Power for the pure hydrogen and diesel-hydrogen engine model, respectively. The spark-ignition turbulent flame model is developed based on [6–8]. This model is able to predict the burn rate for homogeneous charge, SI engines and considers the effects cylinder's geometry, spark locations and timing, air motion, and fuel properties.

Dual-fuel combustion model is a combination of direct-injection diesel multi-pulse model which is designed for modeling CI combustion and spark-ignition turbulent flame model. Using the dual-fuel combustion model, it is possible to predict the combustion rate for a dual-fuel engine where a pilot injection is used to ignite a fuel-air mixture. In this model, the cylinder contents are divided into three thermodynamic zones, each with its own composition and temperature. These three zones are the main unburned zone, the spray zone which contains injected fuel and entrained gas, and the spray burned zone which contains combustion products [9–12].

LFS of the fuel-air mixture is an important input of the combustion model. Our Neural Network LFS model for hydrogen was developed in [13] is used here to estimate LFS value of the hydrogen-air mixture. The combustion model assumes that unburned fuel-air mixture is entrained into the flame front through the flame area at a rate proportional to the sum of the turbulent and laminar flame speeds. The burn rate depends on the amount of unburned mixture left behind the front of the flame. The Spark-ignition turbulent flame model has three calibration parameters: turbulent flame speed multiplier, Taylor length scale multiplier and flame Kernel growth multiplier. These multipliers are used to tune the combustion model using experimental data. These parameters affect the turbulent flame speed value changing the burn rate which affects all of the combustion parameters including in-cylinder pressure trace. The NOx model in this study is similar to our previous studies [14, 15] which is extended Zeldovich. The experimental in-cylinder pressure trace of a single cylinder pure hydrogen engine is used to calibrate the model [16]. Two experimental cases are used to calibrate the model and 1 case was used to validate the model.

For the dual-fuel combustion model, there are four additional calibration parameters. These parameters are entrainment rate multiplier, ignition delay multiplier, premixed combustion rate multiplier and diffusion combustion rate multiplier. These parameters affect the ignition process of the combustion. The calibration parameters of the NOx model are the NOx calibration multiplier and the NOx oxidation multiplier. Here, experimental data from our dual-fuel diesel-hydrogen engine is used to calibrate the model. Similar to the single-fuel hydrogen engine, two experimental cases were used for model calibration and 1 case were used to validate the model. A genetic algorithm similar to [14, 15] is used for in-cylinder pressure trace and $\mathrm{NO_x}$ calibration. Figure. 1 and Figure. 2 show the A schematic of the approach with simulated and experimental in-cylinder pressure trace for the SI single-fuel hydrogen engine is shown in Figure. 1 while CI dual-fuel hydrogen-diesel engine is shown in Figure. 2.

3 Results and Discussion

Experimental data that includes 0.1 crank angle in-cylinder pressure trace and NOx emission for three SI single-fuel hydrogen engine cases [16] and the three CI dual-fuel hydrogen-diesel engine were used to tune the 0D models. One cylinder of a 4.5 liter medium duty Cummins diesel engine [14] was converted to dual-fuel Hydrogen-Diesel engine. No engine boosting was used. The exhaust of the cylinder was separated from the others and the Hydrogen injector is installed in the intake routes of cylinder. A summary of the different cases

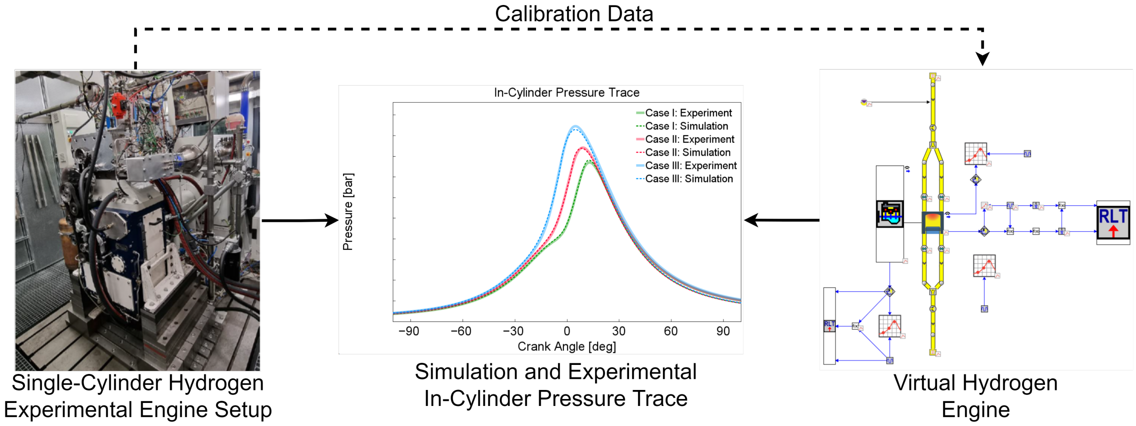

Fig. 1: The spark ignition pure hydrogen engine model development process

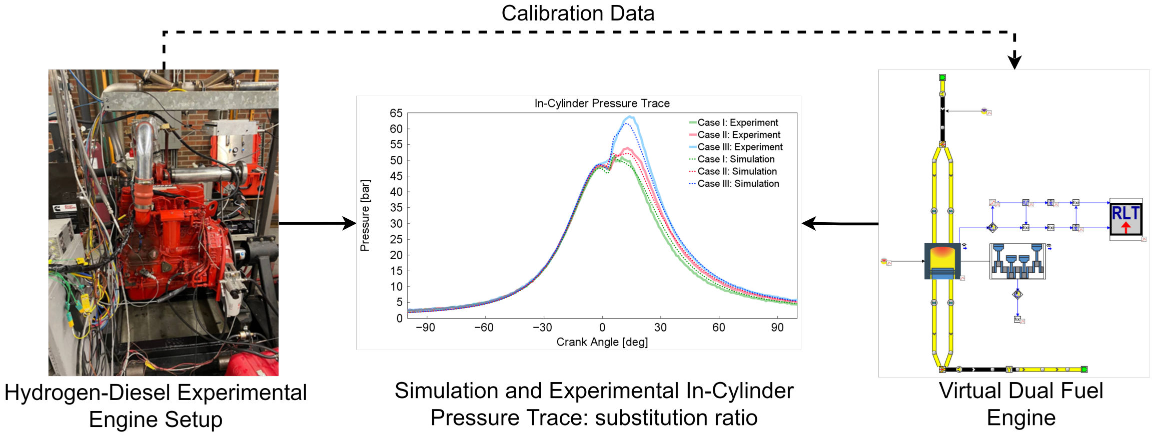

Fig. 2: The hydrogen-diesel CI engine model development process

for the SI single-fuel hydrogen engine and the CI dual-fuel hydrogen-diesel engine are shown in Table 1. Because amount of hydrogen injection is different for different cases they have different lambda values. For the SI engine, hydrogen energy fraction is equal to 1 which means this engine is running on 100% hydrogen for all cases. For the dual-fuel engine, up to 45% of the fuel energy is provided by hydrogen and diesel fuel is the primary fuel.

The experimental and simulation in-cylinder pressure trace for the SI single-fuel hydrogen engine is shown in Figure. 3 while Figure. 4 shows the CI dual-fuel hydrogen-diesel engine. Experiment and simulation for both calibration cases (cases 1 and 3) and the validation case (case2) match quite closely for both engines, indicating that the combustion models and ANN LFS model capture the combustion.

The experimental and simulation NOx emission production are shown for the SI single-fuel hydrogen engine in Figure. 5 and CI dual-fuel hydrogen-diesel engine in Figure. 6. Similar to in-cylinder pressure trace diagrams, the deviation between experimental and simulation NOx emissions are small. The mean relative error in NOx prediction for both single-fuel and dual fuel engines are around 10%. Figure. 6 shows that increasing the hydrogen energy ratio in a dual-fuel engine increases the NOx production. This is attributed to higher combustion temperature which increases NOx formation process. This behaviour is in an agreement with other research [4, 5].

The calculated total flame speed values for the SI single-fuel hydrogen engine and for CI dual-fuel hydrogen-diesel engine are shown in Figure. 7 and Figure. 8. The total flame speed is the summation of LFS and turbulent flame speed. The two combustion models only calculate the LFS between the start of the combustion and exhaust valve opening, so before combustion start and after opening of the exhaust valve the flame speed is set equal

Table 1: Properties of different cases for spark ignition pure hydrogen engine and Compression ignition dual-fuel hydrogen-diesel engine. (cases1 and 3 were used for calibration)

Engine Type	**Case Number**	**Engine Speed (rpm)**	**Hydrogen Energy Ratio (%)**	**Lambda (-)**	**IMEP (bar)**
Spark ignition pure hydrogen engine	Case 1	1080	100	2.378	4.83
	Case 2	1080	100	2.71	4.63
	Case 3	1080	100	2.978	4.51
Compression ignition dual-fuel hydrogen-diesel engine	Case 1	1500	23.5	2.85	5.32
	Case 2	1500	36.5	2.25	6.44
	Case 3	1500	45.4	1.75	7.54

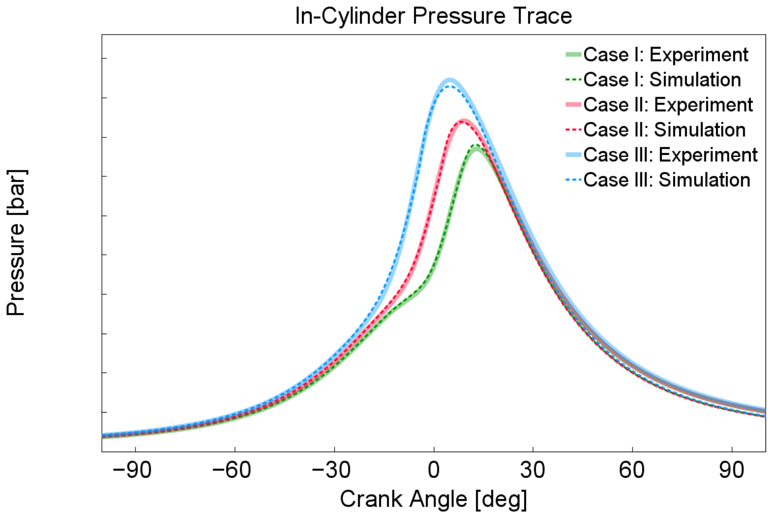

Fig. 3: The experimental and simulation in-cylinder pressure trace for 3 cases for spark ignition pure hydrogen engine. (case 1 and 3 are calibration cases)

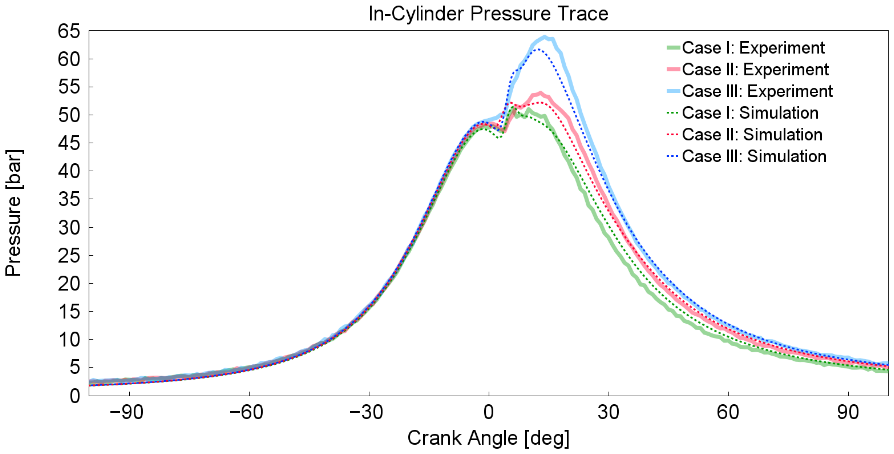

Fig. 4: The experimental and simulation in-cylinder pressure trace for 3 cases for compression ignition diesel-hydrogen engine. (case 1 and 3 are calibration cases)

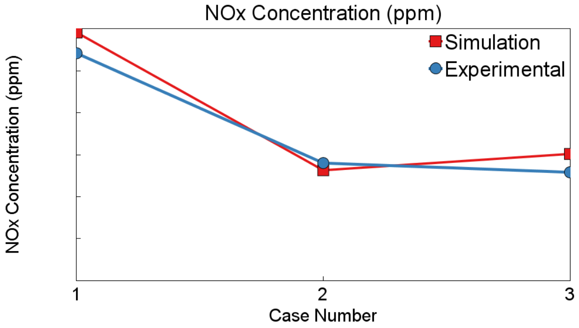

Fig. 5: Experiment data and simulation of NO_x: 3 cases for spark ignition pure hydrogen engine (case 1 and 3 are calibration cases).

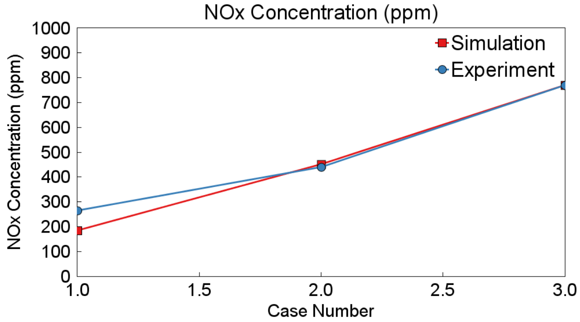

Fig. 6: Experiment and simulation of NO_x: 3 cases for compression ignition diesel-hydrogen engine. (case 1 and 3 are calibration cases)

to zero in Figure. 6 and 8. For SI engines the start of combustion is spark timing, whereas for CI engines it is slightly after diesel fuel injection depends on the injection delay value.

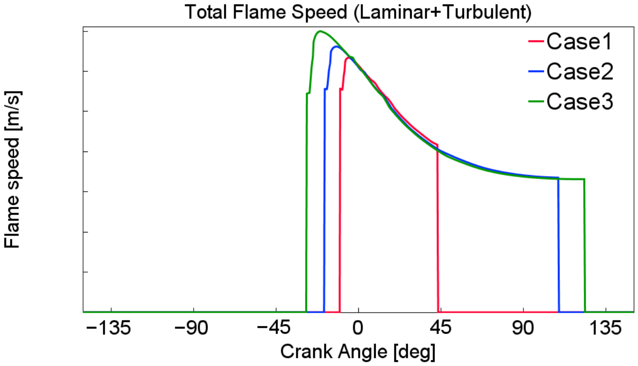

Fig. 7: The total flame speed (laminar flame speed + turbulent flame speed) for 3 cases for spark ignition pure hydrogen engine. (case 1 and 3 are calibration cases)

4 Conclusion

A 0D models for a spark ignition (SI) pure hydrogen engine and a 0D model for compression ignition (CI) dual-fuel hydrogen-diesel engine are incorporated in GT power software. Experimental data for the single-fuel hydrogen and the dual-fuel diesel-hydrogen engines including in-cylinder pressure and NOx emission were used to calibrate the combustion parameters of the models to speed up the simulation. For modeling laminar flame speed (LFS), our ANN model which is a machine learning ANN model was used. Results show that the 0D engine models can accurately model both single-fuel hydrogen and dual-fuel hydrogen diesel engine showing

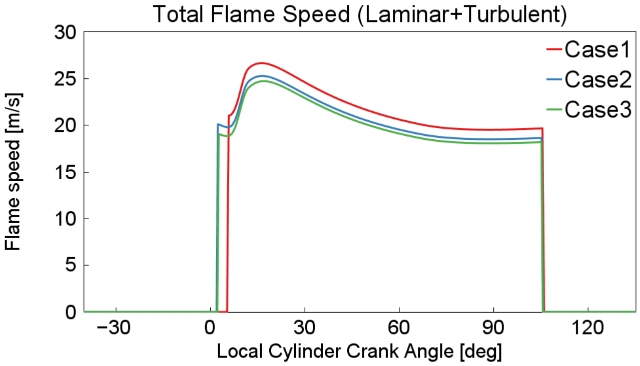

Fig. 8: The total flame speed (laminar flame speed + turbulent flame speed) for for 3 cases for compression ignition diesel-hydrogen engine (case 1 and 3 are calibration cases).

the validity of the developed laminar flame speed in single-fuel and dual-fuel engine modeling. It was also observed that increasing the hydrogen energy fraction in a dual-fuel hydrogen-diesel engine results in higher peak pressure and temperature in the cylinder which increases NOx emissions. The 0D engine platforms for single-fuel hydrogen and dual-fuel hydrogen-diesel engines will be used for future engine calibration and control purposes for these engines.

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