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The effect of hydrogen addition on combustion and emission characteristics of an n-heptane fuelled HCCI engine

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ABSTRACT

The mechanisms of the influence of hydrogen enrichment on the combustion and emission characteristics of an n-heptane fuelled homogeneous charge compression ignition (HCCI) engine was numerically investigated using a multi-zone model. The model calculation successfully captured the most available experimental data. The results show that hydrogen addition retards combustion phasing of an n-heptane fuelled HCCI engine due to the dilution and chemical effects, with the dilution effect being more significant. It is because of the chemical effect that combustion duration is reduced at a constant compression ratio if an appropriate amount of hydrogen is added. As a result of retarded combustion phasing and reduced combustion duration, hydrogen addition increases indicated thermal efficiency at a constant combustion phasing. Hydrogen addition reduces indicated specific unburned hydrocarbon emissions, but slightly increases normalized unburned hydrocarbon emissions that are defined as the emissions per unit burned n-heptane mass. The increase in normalized unburned hydrocarbon emissions is caused by the presence of more remaining hydrocarbons that compete with hydrogen for some key radicals during high temperature combustion stage. At a given hydrogen addition level, N_2O emissions increases with overly retarding combustion phasing, but hydrogen addition moderates this increase in N_2O emissions.

1. Introduction

Hydrogen is a clean fuel whose combustion does not generate carbon dioxide, particulate matter (PM) and unburned hydrocarbons (HC). It has been shown that hydrogen provides satisfactory performance in internal combustion (IC) engine applications, although there are various challenging issues [1–4].

Unfortunately hydrogen is an energy carrier and has to be obtained from hydrocarbon fuels or water. The use of pure hydrogen as a primary fuel for internal combustion engines is still too expensive today. Alternatively, hydrogen enrichment, i.e. use of a small amount of hydrogen as additive to conventional fossil fuels, may be a more practical way to apply hydrogen. Previous studies have shown that hydrogen enrichment helps to extend lean flammability limits and to increase flame speeds of hydrocarbon fuels [5,6]. As a result, the addition of hydrogen to a spark-ignition (SI) engine extends the lean operational limits and thus allows the engine to operate at leaner conditions with reduced NO_x emissions [7,8].

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Homogeneous charge compression ignition (HCCI) combustion has been attracting more and more attention from scientists and engineers due to its potential to virtually eliminate NO_x and PM emissions from engine combustion. The effect of hydrogen enrichment on the performance of HCCI combustion has also been investigated by many researchers. Shudo et al. [9–11] investigated the effect of hydrogen enrichment on HCCI combustion of dimethyl ether and found that the addition of hydrogen retarded the combustion phasing. On the other hand, the addition of hydrogen to a natural gas fuelled HCCI engine has been shown to advance combustion phasing and to extend the lean operational limits [12–15]. Checkel et al. [14–18] investigated the effect of reformer gas (hydrogen rich gas) enrichment on iso-octane and n-heptane fuelled HCCI combustion and found that the effect depended on the octane number of the base fuel.

Diesel engines are widely used in transportation and off-road vehicles. The advantages of HCCI combustion make it a potential alternative combustion mode to conventional diesel engines [19]. Diesel fuels usually have two-stage combustion, a low temperature heat release (LTHR) stage that initiates the ignition process and a primary high temperature heat release (HTHR) stage. One issue with diesel HCCI combustion is the earlier ignition that limits the maximum compression ratio and thus the fuel conversion efficiency [20]. Appropriate combustion phasing (ignition timing) and reasonable combustion duration are crucial for a diesel HCCI engine to obtain higher fuel conversion efficiency and lower pollutant emissions [20,21]. Hydrogen is a fuel with higher auto-ignition temperature which may help to control the combustion phasing of a diesel HCCI engine. Meanwhile, hydrogen has a higher flame speed and leaner extinction limit, suggesting that the addition of hydrogen may enhance the primary high temperature combustion process and thus reduce the combustion duration of a diesel HCCI engine. Our experimental measurements [22] show that hydrogen enrichment does help to retard the combustion phasing, reduce the combustion duration and improve the fuel conversion efficiency of a diesel fuelled HCCI engine. However, not enough attention has been paid for the fundamental mechanisms behind the phenomena of hydrogen enriched HCCI combustion in Ref. [22] and other previous publications.

This paper further investigates the effect of hydrogen enrichment on the combustion and emission performances of an HCCI engine fuelled by n-heptane, a primary reference fuel of diesel, numerically by a multi-zone model with relatively detailed chemistry. Being different from Ref. [22], this paper focuses on the fundamental mechanisms associated with hydrogen enrichment of HCCI combustion. The paper starts with the brief description of the numerical model and the studied engine, followed by the presentation and analysis of results. Finally, concluding remarks are drawn.

2. Numerical model

The studied engine is a Cooperative Fuel Research (CFR) engine used in the experimental study in Ref. [22]. It is a single-cylinder, four-stroke, variable compression ratio engine. The basic engine specifications are listed in Table 1. A port fuel injector that is the same as that employed in Ref. [23] was used to atomize and inject n-heptane just upstream of the intake port. Hydrogen was introduced to the intake port after the injection of n-heptane. More details about the engine can be found from Ref. [22].

A multi-zone model was employed to do the simulation. It assumes the working fluid to be an ideal gas and simulates a full four-stroke cycle of engine operation, starting from top dead centre (TDC) during the exhaust stroke and finishing at the same point after the intake, compression, combustion and exhaust strokes, i.e. from −360° to 360° after top dead centre (ATDC).

Eight zones were used in the model, including one crevice zone, one boundary zone and six core zones. The model assumes that the temperature of the crevice zone is always lower than or equal to the cylinder wall temperature due to the large ratio of surface area to volume. The volume of the crevice zone was assumed to be constant as 2% of the clearance volume of the investigated engine. The mass distribution in the boundary zone and core zones was assumed to be a normal distribution.

Heat transfer between working fluid and cylinder wall is assumed to happen through the boundary zone due to convection in the model. Each zone exchanges heat with its neighbouring zones due to conduction and with cylinder wall due to radiation. There is mass exchange between crevice zone and other zones if pressure and temperature changes. To simplify the calculation, the mass exchange has been neglected during each time step. However, a mass adjustment is conducted after each time step. Then the adjusted masses are used during the next time step. The mass adjustment is conducted based on the total mass inside cylinder and the mass in the crevice zone. Before and after each time step, the mass of crevice zone can be calculated by the ideal gas state equation according to the crevice zone temperature, volume, composition and cylinder pressure. Then the adjusted crevice zone mass Δm_{cre} can be obtained. During the pressure increase process, fluid flows from boundary zone and core zones to crevice zone, i.e. Δm_{cre} is positive. Oppositely, Δm_{cre} is negative during the pressure decrease (expansion) process. More details of the multi-zone model can be found elsewhere [24] and from the Supplementary material that provides all details, governing equations and related references for the model.

Table 1 – Engine specifications.

Cylinder bore	8.255 cm
Stroke	11.43 cm
Displacement volume	611.7 cm^3
Connection road length	25.4 cm
Compression ratio	6–16
Combustion chamber	Pancake shape, flat top piston
Intake valve open	10°CA ATDC[a]
Intake valve close	34°CA ABDC
Exhaust valve open	40°CA BBDC
Exhaust valve close	5°CA ATDC
Fuel system	Air-assisted port fuel injection

a ATDC: after top dead centre.