ENABLING EFFICIENT, AFFORDABLE AND ROBUST USE OF RENEWABLE HYDROGEN IN TRANSPORT AND POWER GENERATION

Mid-term Knowledge Sharing Report

Funding Agreement Details

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1. Project summary and scope

This project aims to demonstrate the performance and value of highly efficient, reciprocating engines operating on renewable hydrogen. This includes the use of novel spark and compression ignition engine systems coupled with other advanced technologies. These engines are currently being developed through first and second-generation prototypes informed by more fundamental experiments and numerical modelling.

The key activities of this project are as follows.

(a) the Pressurised Flow Reactor (PFR) Programme aims to develop chemical kinetic models of hydrogen autoignition to be used in the High-Performance Computation (HPC) programme;

(b) the Constant Volume Combustion Chamber (CVCC) Programme aims obtain comprehensive optical measurements of the fuel jet and the flame, thereby forming a validation database for the HPC programme;

(c) the Cooperative Fuel Research (CFR) Engine Programme aims to show definitively how hydrogen's autoignition and combustion properties limit how aggressively engines can be designed for high efficiency;

(d) the HPC Programme will employ advanced, computational fluid dynamic simulations to provide fundamental understanding of hydrogen injection, ignition, and combustion;

(e) the Spark-ignition (SI) Engine Programme aims to demonstrate SI engine efficiency of at least 45%;

(f) the Compression-ignition (CI) Engine Programme aims to demonstrate CI engine efficiency of at least 45%;

(g) the Techno-economics Programme employs state-of-the-art techno-economic modelling to demonstrate the value of highly efficient, reciprocating engines in different systems that either generate, transport or use renewable hydrogen.

This report presents an update on the activities undertaken at the mid-point of this project. This includes our progress in programmes (a), (b), (e) and (f) above.

2. Progress update

2.1 The PFR Programme

In this programme, the combustion chemistry of hydrogen was studied both experimentally and numerically. First, the oxidation of hydrogen near its second explosion limit was investigated in a turbulent flow reactor at pressures up to 10 bar, temperatures of 950 K and an equivalence ratio of 0.035. These experiments demonstrated evident negative pressure dependence from roughly 1 to 4 bar, with further increases in pressure resuming its positive impact on reaction rates. The simulated and measured species concentrations along the reactor generally agreed within a factor of 2, suggesting a need for the improvement of the existing combustion kinetic models of hydrogen.

Given this *characterisation* of hydrogen autoignition, further investigation was therefore conducted to measure the rate coefficient of an elementary reaction $H + O_2 (+ M) = HO_2 (+M)$ (R2), which is one of the most sensitive reactions in hydrogen's combustion chemistry at these conditions. The rate coefficients were obtained at 950 – 1010 K. Combined with literature results, an Arrhenius expression was proposed, $k_{2,0} = 4.50\times10^{20} (T/K)^{-1.73}$ [$\mathrm{cm}^6\ \mathrm{mole}^{-2}\ \mathrm{s}^{-1}$], for the reaction rate at the low-pressure limit over 500 K – 2000 K with N_2 as the bath gas. Simulations using the kinetic models adopted with the proposed Arrhenius expression for this reaction then demonstrated improved agreement with the experiments.

2.2 The CVCC Programme

In this programme, a single-hole, high-pressure hydrogen injector and high-pressure fuelling system were developed to enable hydrogen fuel-jet and flame experiments in the CVCC facility. The H_2 injector can be operated at up to 200 bar injection pressure, featuring a modified commercial gasoline injector assembled with an external nozzle to form a single coaxial jet for experiments in the canonical CVCC configuration.

The steady hydrogen flow rate, nozzle discharge coefficient, nozzle pressure-ratio, and jet penetration were characterised using two schlieren setups with the image resolution adapted to the size of the features that were investigated. The applicability of existing jet penetration models under engine relevant pressure was validated.

The resulting hydrogen flames were also optically measured. Considerable differences to the characteristics of hydrocarbon flames were observed; the jet tends to ignite in the recirculation zone upstream of the jet-head with large stochastic variability of the ignition delay. Following ignition, the flame rapidly encloses the whole jet volume and stabilizes close to the injector.

The dataset obtained reports high-fidelity information of hydrogen jet behaviour in a canonical configuration under engine-relevant conditions. It provides critical input for a range of modelling efforts, including validation of hydrogen autoignition models, validation of 3D numerical calculations (the HPC programme), and provides information on high-pressure hydrogen jet mixing.

2.3 The SI Engine Programme

In the first phase of this programme, an experimental and numerical study of a prototype, integrated, direct injection (DI), spark-ignition (SI) system for hydrogen fuelling was conducted in a base diesel engine. The results demonstrated knock-limited performance exceeding 40% indicated thermal efficiency on this high compression ratio engine over a wide range of air-to-fuel ratios. Specifically, the inferred burn profiles at knock-limited conditions highlighted significantly retarded combustion compared to that of a typical SI engine operating at its peak efficiency. Results also indicated that the hydrogen burn rate falls significantly at leaner conditions, ultimately leading to significant unburned fuel fraction, combustion variability and low thermal efficiency.

Subsequent kinetic simulations suggested that some plausible combination of residual nitric oxide (NO) and locally high charge temperatures at intake valve closing (IVC) could lead to autoignition at the knock-limited conditions identified in the experiments. This gave confidence in the kinetic modelling, prompting a parametric study of hydrogen autoignition. The results of this study presented pathways to avoid engine knock and attain high thermal efficiencies, which will be explored in the remainder of this project with the second-generation SI engine.

2.4 The CI Engine Programme

A set of modifications of the existing CI engine test-rig was conducted to enable the novel CI hydrogen engine concept utilizing a dual direct-injection hydrogen-diesel mode (H2DDI). These modifications included an adaptation of the engine cylinder head to fit two injectors for hydrogen and diesel as well as the development of a high-pressure hydrogen fuelling system. This unoptimized engine configuration was assessed in the terms of engine performance, emissions, and attainable energy substitution of diesel fuel with hydrogen.

The study employed the energy substitution approach at a constant engine fuelling rate. A wide variation of hydrogen injection timing from during the intake stroke up to shortly before top dead centre was tested to highlight the importance of hydrogen charge stratification and residence time to avoid pre-ignition. Up to 50% substitution with hydrogen on an energy basis was possible for late hydrogen injection without pre-ignition, compared to previously reported attempts using H_2 port fuel injection that were only able to achieve about 20% substitution at comparable conditions. Indicated thermal efficiencies in the range of 40-45% with only moderately increased nitrogen oxide emissions were also observed.

The second-generation CI engine, to be developed and tested in the remainder of the project, will aim at faster injection and higher efficiency by tailoring the combustion phasing and reducing the wall heat losses through charge stratification while simultaneously avoiding pre-ignition.

3. Key highlights and difficulties experienced

3.1 The PFR Programme

Key highlights:

- the results demonstrated the importance of pressure on hydrogen autoignition;
- an innovative approach to examining the kinetics of a key reaction was employed, and this enabled improvement to an existing kinetic model over a range of pressures experienced in engines.

Programme-specific challenges:

- Developing a turbulent flow reactor for high-pressure and high temperature experiment was a challenge overall. The initial idea of using nitrogen as the dilution gas to control the reaction rates was replaced by using air due to the limited supply capacity and high operational cost. The impact of the excess oxygen on reaction rates was counted in kinetic simulation and overall was well-captured by existing models.
- Quantitative analysis of water from hydrogen oxidation was a challenge as well. Producing a calibrating curve with a range of known water vapor concentrations was not straightforward, particularly considering the potential water condensation in the sample line. After calculation, we found that water fraction in fully oxidized hydrogen is lower than that in saturated air at ambient temperature. We then used a refrigeration unit and bubbled air through a bottle of water immersed in a water bath cooled by the unit. A calibration curve for water quantification was thus obtained.

3.2 The CVCC Programme

Key highlights:

- a single-hole, high-pressure hydrogen injection system was developed to enable hydrogen fuel-jet and flame experiments;
- hydrogen jet was found to ignite in the recirculation zone upstream of the jet-head with large stochastic variability of the ignition delay;
- it was also found that following ignition, the flame rapidly encloses the whole jet volume and stabilizes close to the injector.

Programme-specific challenges:

- High-pressure hydrogen injectors capable of handling injection pressure exceeding 200 bar are not commercially available on the market, which prompted custom modification of a commercial injector to achieve the desired pressure capacity and flow-rate.

- The supply system and piping for high-pressure hydrogen had to be customized and the safety concerns prompted an external, certified company for the final installation. This process proved time-consuming, which resulted in delays in the programme. However, the challenge was successfully overcome.

3.3 The SI Engine Programme

Key highlights:

- the first-generation SI engine with an integrated injection and ignition system was designed, built and commissioned;
- an indicated thermal efficiency above 40% was achieved;
- it was shown that some plausible combination of residual nitric oxide (NO) and locally high charge temperatures at IVC could lead to autoignition, and hence knock-limited engine performance at high compression ratios.

Programme-specific challenges:

- Given the space limitations in the engine head, the design and fabrication of an integrated fuel injection and ignition system proved challenging. One particular challenge was associated with packaging the integrated system so that minimal head modification was required. This led to the design of a complex fuel passage, which could not be fabricated by conventional machining. Therefore, 3D metal printing technology was used for its fabrication.
- Given the high compression ratio of the base diesel engine, engine knock under hydrogen-fuelled operation was another major challenge experienced. This limited the attainable peak thermal efficiency in the first-generation engine. To address this, a series of modifications are in progress to lower effective compression ratio and avoid engine knocking.

3.4 The CI Engine Programme

Key highlights:

- fifty percent hydrogen substitution was achieved in this program, which is about twice as high as other dual-fuel CI engine technologies;
- indicated thermal efficiencies in the range of 40-45% with only moderately increased NO emissions were observed;
- a pathway was presented to achieve a higher energy substitution rate by increasing the hydrogen injection rate using a custom injector nozzle geometry, with the potential to additionally increase the efficiency through charge stratification.

Programme-specific challenges:

- Given the high compression ratio of the base engine, hydrogen substitution rate was limited by pre-ignition. Modifications to the injector configuration and its flow rate are currently being implemented in the second-generation engine to overcome this problem. This includes late injection of hydrogen using an injection unit with a higher flow rate.

- High NO_x emissions was another major challenge when the engine was operating on hydrogen. This will be mitigated by exhaust gas recirculation and modifying injector configuration in the second-generation engine.

4. Commentary on commercialisation prospects (including for example, product costings, business model and preliminary market assessment)

Not yet applicable.

5. Summary of knowledge sharing activities completed (e.g. publications, conferences, patents)

Below is the summary of publications completed by the mid-point of this project.

1. Lu Z., Yang Y., Lacey J., Brear M., "Experimental and numerical analysis of hydrogen oxidation in a flow reactor, " *Proceedings of the Australian Combustion Symposium*, Dec. 2019;
2. Lu Z., Jiang J., Yang Y., Lacey J., Brear M., "Hydrogen oxidation near the second explosion limit in a flow reactor, " *accepted for presentation at the 38th International Symposium on Combustion*, PROCI-S-19-01209, 2020;
3. Mortimer J., Yoannidis S., Poursadegh F., Lu Z., Brear M., Yang Y., Etherington D., Heijkoop M., Lacey J., "An experimental and numerical study of a hydrogen fuelled, directly injected, heavy duty engine at knock-limited conditions, " *accepted for presentation at the ASME Internal Combustion Engine Fall conference*, ICEF2020-2920, Nov. 2020.
4. Yip H.L., Srna A., Liu X., Kook S., Hawkes E.R., Chan Q. N., "Visualization of Hydrogen Jet Evolution and Combustion under Simulated Direct-Injection Compression-Ignition Engine Conditions, " *submitted to the International Journal of Hydrogen Energy* on 17/7/2020;
5. Liu X., Srna A., Yip H. L., Kook S., Chan Q. N., Hawkes E. R., "Performance and emissions of hydrogen-diesel dual direct injection (H2DDI) in a single-cylinder compression-ignition engine," *submitted to the International Journal of Hydrogen Energy* on 17/7/2020;
6. Liu X., Srna A., Yip H. L., Kook S., Chan Q. N., Hawkes E. R., "Comparison of hydrogen port injection and direct injection (DI) in a single-cylinder dual-fuel diesel engine," *submitted to the 22nd Australasian Fluid Mechanics Conference* on 19/7/2020.

6. Acknowledgement

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