

Most research of hydrogen use in internal combustion engines (ICEs) has revolved around spark ignition (SI) engines. The great interest in SI hydrogen engines was not solely academic. In fact, large automakers such as Ford, DaimlerChrysler and BMW developed hydrogen fueled models. On the other hand, hydrogen use in compression ignition (CI) engines has not been particularly attractive and one of the main reasons is hydrogen's high autoignition temperature.

To tackle hydrogen's high resistance to autoignition, three strategies have been proposed. Firstly, the use of very high compression ratios (>29:1). This approach is not attractive because it results in problems related to the mechanical strength of the engine structure, therefore, it requires an engine redesign. Secondly, the use of a glow plug with the purpose of preheating the intake air or the hydrogen/air charge. This technique is generally simple and has been reported to lead to very low NO<sub>x</sub> emissions and higher fuel efficiency and power to weight ratio compared to the conventional, diesel-fueled mode. Despite these promising results, the increase of the intake air temperature when used without any substantial modification of a conventional CI engine, leads to a decrease of the volumetric efficiency which results in the decrease of the indicated mean effective pressure (IMEP), the indicated thermal efficiency and the brake thermal efficiency. The third approach encompasses a dual fuel strategy, where the ignition of the in-cylinder charge is achieved by the direct injection of a more reactive fuel, e.g., diesel. This approach is particularly attractive, because it offers a unique flexibility in the engine operation while also maintaining (at least to some extent) the benefits from the CI/HCCI mode. In CI/HCCI dual-fuel operation, hydrogen has been mainly used (so far) with carbon-based fuels, such as (bio-)diesel, natural gas and others. Being carbon-based, the fuel blends produce carbonaceous emissions (e.g., CO<sub>2</sub>) directly or indirectly, thus, cancelling or reducing the efforts for drastic greenhouse gases (GHG) reduction.

In the current work, an alternative approach is proposed and explored numerically; the use of hydrogen peroxide as an ignition promoter. The idea of using hydrogen peroxide for propulsion purposes is not actually new and dates back to the 1930s when it was first used as a rocket fuel. Since then, its use as a fuel has mainly been limited to aerospace and military applications. In academic research hydrogen peroxide has been used as an ignition promoter in engine experiments (i.e., for the same purpose as in the current work) with fuels like diesel, jatropha oil and. Apart from the fact that it can be produced from renewable sources, hydrogen peroxide has also the advantage that there is an existing logistics mechanism available to support its production, storage and distribution. The reason for this, is because it is a substance used for other purposes besides as a fuel: medical use as an antiseptic, domestic use as a cleanser and disinfectant, and in the food sector for processing and bleaching certain foods, to name only few applications.

The aim of the current work was to explore the potential and identify the limitations of a H<sub>2</sub>/H<sub>2</sub>O<sub>2</sub> fuelled CI engine with water/steam dilution in view of engine performance characteristics using simplified CI-type engine model setups. The current project is meant to be a stepping stone towards the development of a new technology that will enable the rapid decarbonisation of HDVs and ships.

In the first part of the current work, a simplified zero-dimensional HCCI numerical model was used in order to explore the feasibility of using hydrogen in a dual fuel concept where hydrogen peroxide acts as ignition promoter [1]. The analysis focused on the engine performance characteristics, the combustion phasing and NO<sub>x</sub> emissions. It was shown that the use of hydrogen/hydrogen peroxide at extremely fuel

lean conditions ( $\phi_{eff} = 0.1 - 0.4$ ) can result in significantly better performance characteristics (up to 60% increase of IMEP and 80% decrease of NO<sub>x</sub>) compared to the case of a preheated hydrogen/air mixture that aimed to simulate the use of a glow plug. It was also shown that the addition of H<sub>2</sub>O<sub>2</sub> up to 10% (per fuel volume) can increase significantly the IMEP, power, torque, thermal efficiency (reaching values more than 60%) while also decreasing remarkably NO<sub>x</sub> emissions which would not require any exhaust after-treatment, for all engine speeds. Next, the same numerical HCCI model was used to investigate the addition of hydrogen peroxide along with steam at various fuel lean conditions ( $\phi_{eff} = 0.2 - 0.6$ ) and compression ratios (15–20) [2]. The use of hydrogen peroxide as an ignition promoter demonstrated increased IMEP (16%–39%), thermal efficiency (up to 2%), and reduced NO<sub>x</sub> (50%–76%) when compared to the conventional method of intake charge heating. When hydrogen peroxide was used as an ignition promoter, a 15% addition of steam was sufficient to reduce NO<sub>x</sub> by 93%–97%, though this reduced IMEP and thermal efficiency slightly. When heat transfer was considered and steam addition was increased from 0%–10%, no increase in intake air heating was able to match the IMEP of 5% hydrogen peroxide addition without an increase in the equivalence ratio (up to 40%). The parametric space of hydrogen peroxide (0%–25%) and steam (0%–40%) addition was explored in view of engine performance metrics, showing the complete range of conditions possible through control of both inputs. A three-order reduction in NO<sub>x</sub> was possible through steam addition. An optimal balance of performance and emissions occurred at 5%–10% hydrogen peroxide and 10%–15% steam addition.

In the second part of the project a zero-dimensional, time dependant compression ignition engine model was developed. Unlike the first part which revolved around the HCCI mode, this part of the project concerned a more conventional CI engine mode. The model accounted for aspects such as the engine specifications, the volume change, the vaporisation of the injected fuel, the time of the injected fuel, the duration of the fuel injection, as well as the thermophysical properties of the initial in-cylinder charge (hydrogen/air). The combustion model was created using datasets from HCCI engine simulations with detailed chemistry. This enabled the establishment of a simplified, reduced order Weibe function to represent the combustion reaction progress. Parameters for the Weibe function were adaptable and were calculated based on the hydrogen peroxide in the combustion mixture. This allowed the model to simulate different combustion properties for each case studied. Using this simplified model, it was predicted that a timed injection of a 6%mol hydrogen peroxide solution could favourably control the combustion reaction and improve the engine's IMEP by 12% compared to the HCCI case.

### References:

- [1] Dimitrova, I. D., Megaritis, T., Ganippa, L. C., Tingas, E. A. (2022). Computational analysis of an HCCI engine fuelled with hydrogen/hydrogen peroxide blends. *International Journal of Hydrogen Energy*, 47(17), 10083-10096.
- [2] Fernie, O., Megaritis, T., Ganippa, L. C., Tingas, E. A. (2022). Numerical analysis of zero-carbon HCCI engine fuelled with steam diluted H<sub>2</sub>/H<sub>2</sub>O<sub>2</sub> blends. *Fuel*, 326, 125100.