Hydrogen-powered internal combustion engines (H_2-ICEs) offer a promising pathway for decarbonizing the transport sector, particularly in hard-to-abate segments such as heavy-duty and off-road applications. In addition to enable a clean andCO_2-free combustion process, this technology benefits from the well-established maturity of manufacturing processes and facilities, as well as of a seamless integration into existing powertrains. The need to reduce development costs and time-to-market has led many OEMs to develop the first generation of H_2 ICEs using their current diesel engines as a reference, because of their high mechanical strength. However, this layout is not the most suitable for hydrogen operation, primarily due to the predominant swirl motion, which impairs hydrogen distribution and fails to enhance turbulence generation, a key factor in promoting fast and stable combustion processes.

In this context, numerical simulations serve as a powerful tool to accelerate and support system development by providing insights that cannot be obtained solely through experimental testing. This work presents the main stages of the conversion of a state-of-the-art 2.4L diesel engine for direct-injection hydrogen operation, including a comprehensive numerical analysis and experimental testing. Initially, 0D/1D-CFD analyses were conducted to identify the optimal compression ratio, select the boosting system, and optimize valve timing and lift profiles. Subsequently, 3D-CFD simulations were performed to refine the hydrogen-air mixture formation process. A sensitivity analysis on injection timing was first carried out to determine the optimal injection window, capable of maximizing mixture homogeneity while minimizing volumetric efficiency losses and hydrogen backflow. Next, various spray injector guiding caps were evaluated to assess their influence on in-cylinder dynamics and mixture properties. Finally, the impact of swirl intensity on hydrogen distribution was examined by modifying the eccentricity of the intake valve seats. The optimization of the combustion chamber geometry resulted in significant improvements in mixture homogeneity. A flamelet-based combustion model was subsequently improved for modeling hydrogen combustion. Indeed, due to hydrogen's low Lewis number, premixed hydrogen-air flames in lean conditions exhibit strong thermodiffusive instabilities, making the numerical simulation of the combustion process particularly challenging. The intensity of these instabilities is influenced by thermodynamic parameters, such as mixture temperature, pressure, and dilution rate, leading to substantial variations in combustion behavior across different operating conditions. Consequently, these effects must be properly accounted for not only to ensure model robustness but also to enhance accuracy across a wider range of operating conditions. In the 3D-CFD environment, two sets of lookup flame speed maps were implemented: laminar flame speed (S_L) maps derived from standard 1D-CFD simulations in homogeneous reactors and freely propagating flame speed (S_M) maps that account for the effects of thermodiffusive instabilities. The model employing S_L maps required recalibration of combustion model parameters when changing the dilution rate to maintain consistency with experimental data. Conversely, the model utilizing S_M maps demonstrated remarkable accuracy across different air-to-fuel ratios without necessitating parameter recalibration, highlighting the critical role of thermodiffusive flame instabilities in the combustion process. Based on these findings, the impact of such instabilities was evaluated throughout the entire combustion process from both global and local perspectives. The relevance of thermodiffusive instabilities was observed to increase with the air-to-fuel ratio, thereby enhancing combustion speed in leaner mixtures. Additionally, the implementation of thermodiffusive instabilities influenced the preferred flame propagation direction, as stronger instabilities were identified in the leanest and lowest-temperature regions of the flame front.

The results of the numerical analysis were used to built a physical prototype, whose performances were subsequently evaluated on the dynamic test bench. The developed engine concept successfully achieved performance levels comparable to the base engine while maintaining limited engine-out NOx emissions. Finally, the engine was tested on the Large Spark Ignition Nonroad Transient Cycle, and the resulting engine-out NOx emissions were found to be below the regulatory threshold.