

# Summary

In the current context of research of technological solutions to transition away energy systems from fossil energy sources dependency, the transportation system is facing significant challenges. Despite electrification has emerged as a potential solution, the technological limitations and the concerns related to intermittency of renewable energy sources, supply chain security, and socio-economic costs highlight the need for a diversified approach that leverages multiple energy sources and integrates existing technologies. Among the viable alternatives, hydrogen-fueled internal combustion engines (H<sub>2</sub>ICEs) are gaining momentum due to their robustness in challenging environmental conditions, tolerance to hydrogen purity variations, and high efficiency under heavy loads. Additionally, H<sub>2</sub>ICEs can leverage synergies with existing manufacturing processes and supply chains, making them an attractive pathway for decarbonizing hard-to-abate sectors.

Although internal combustion engine technology is well-established, adapting these engines for hydrogen presents unique challenges. Converting existing engines to operate with hydrogen offers a cost-effective alternative for developing entirely new platforms but requires thorough selection of hydrogen-specific components to ensure optimal performance, efficiency, and emissions control. To support this transition, numerical simulations play a crucial role in providing reliable preliminary analyses during the development phase.

This study focuses on the development of a virtual analysis methodology, combining numerical and experimental outcomes, to assess the potentialities of a new generation of hydrogen engines derived from a current production 12.9 L NG engine for heavy-duty applications. In order to fully exploit the potential of lean combustion, a preliminary optimization of the subsystem components has allowed to select the turbocharger architecture able to deal with the significant increase of air needed to reach this target. Once assessed the performance potential in terms of achievable engine load, a wide experimental campaign was performed to characterize hydrogen combustion process of two different concepts: a PFI version, aiming at testing the most straightforward conversion pathway, and the DI version, which represent the subsequent step to reach higher performance. The outcomes of this analysis, focused on assessing the impact of the main calibration parameters on combustion process in terms of efficiency, combustion stability and NO<sub>x</sub> emissions, have verified the significant role of mixture inhomogeneity in limiting the performances of DI concept, and the relevance of a proper selection of combustion timing to guarantee stable operations, even under particularly lean conditions. Afterwards, these outcomes were integrated within a phenomenological 1D-CFD combustion model based on the entrainment and burn-up approach. A key enhancement of the model

was the implementation of a correlation to modify the laminar-to-turbulent transition based on mixture conditions, considering both experimental evidence and theoretical considerations related to the low Lewis number of hydrogen-air lean mixtures. Experimental data were used to validate the model for both engine configurations.

Finally, the model was extended with a NO<sub>x</sub> sub-model, enabling emissions estimation in virtual investigations. The potentialities of the model to reproduce different operating conditions are discussed, as well as the main limitations and the possible actions to improve its predictive capabilities