## **Abstract**

Optimising existing internal combustion (IC) engines remains a key engineering priority in the areas of fuel economy, utilisation of alternative fuels, and exhaust emissions reduction as the emission standards continue to become stringent worldwide. The optimisation of IC engines requires the evaluation of their performance parameters and exhaust emissions under transient conditions as found during actual driving cycles. However, physical testing on test benches is both costly and time-consuming, creating a need for reliable, real-time simulation tools supporting the development of modern IC engines.

This work introduces a simulation toolchain framework for real-time transient engine simulations. The toolchain integrates a 0D Stochastic Reactor Model (SRM) with tabulated chemistry into Model-in-the-Loop (MiL) and Hardware-in-the-Loop (HiL) platforms using the Functional Mock-up Interface (FMI) standard. By encapsulating the SRM within a Functional Mock-up Unit (FMU), the framework enables cross-platform simulations, bridging the gap between physical modelling accuracy and practical applicability in engine development workflows. The developed toolchain enables real-time transient engine simulations in MiL/HiL platforms and in stand-alone mode, and is considered a physics-based driving cycle simulator. It can simulate engine-out emissions and performance parameters under driving cycles such as the Worldwide harmonised Light vehicles Test Procedure (WLTP) and the Non-Road Transient Cycle (NRTC). Through the use of an Artificial Neural Network (ANN)-based meta-model of the driving cycle simulator, the computational cost of simulations has been reduced well below real-time, while maintaining the accuracy of the physicsbased model. The FMU-based structure allows seamless integration with different models of exhaust after-treatment systems, enabling full-path simulation from combustion to tailpipe emissions.

The toolchain was applied in both stand-alone mode and integrated MiL/HiL environments for Compression-Ignition (CI) and Spark-Ignition (SI) engines under transient driving conditions of WLTP and NRTC. The investigations for SI engines focused on simulating engine performance parameters and exhaust emissions during the cold-start phase of the driving cycle for engines fuelled with compressed natural gas. Applications for CI engines dealt with predicting driving-cycle to driving-cycle variability in exhaust emissions, including CO<sub>2</sub>, NO<sub>x</sub>, soot, unburned hydrocarbons and CO. The toolchain's application in MiL and HiL configurations was validated on the dSPACE system and demonstrated seamless integration into real-time development environments. The capability of co-simulation with after-treatment models was verified based on the coupling with a selective catalytic reduction catalyst model applied to simulating an ammonia-biodiesel-fuelled engine. Overall, results obtained from different applications indicate the strength and versatility of the toolchain developed for studying engine behaviour under transient conditions, where details of emissions formation and fuel effects are of importance. The developed tool can be applied for engine certification studies or calibration and further contribute to the development of virtual test benches or digital twins in both research and industrial contexts.