The growing concern about the transportation industry pollution effects on the environment and on the human health has pushed the governments worldwide to adopt more stringent emissions standards and severe type approval procedures, representative of the real vehicle usage. With the newly introduced test procedures, which includes more energy-demanding driving cycles such as the Worldwide harmonized Light vehicles Test Cycles (WLTC) and the Real Driving Emissions (RDE) test cycle, engine emissions have to be controlled under a broader range of operating conditions, including low temperature and highly transient driving manoeuvres. In this scenario, the adoption of the after-treatment systems has become essential, in both spark and compression ignition engines, to comply with the emissions targets.

In particular, compression ignition engines require the combination of different after-treatment devices to perform the selective abatement of different pollutants species, such as CO, unburned HydroCarbons (HC), Nitrogen Oxides (NO_x) and Particulate Matter (PM), in a wide range of operating conditions, including at low temperature. Moreover, the emissions abatement must be guaranteed for the useful life of the vehicle, thus introducing additional constraints in the design of the after-treatment system.

In this context, the automotive industry demands for robust modeling methodologies and flexible simulation tools to support the vehicle engineering process, reducing the number of costly and time-consuming experimental campaigns and thus the time-to-market of the engine.

In this research work, different modeling approaches were explored ranging from detailed multi-dimensional models, suitable for component-level analysis and optimization, to mono-dimensional models suitable to perform system-level performance assessment, optimization and controls development. The aim of this research work was to develop robust methodologies to predict the conversion efficiency of complex after-treatment systems for the future generation of diesel powertrains, with a comprehensive approach and compassing both component- and system-level optimization to assess the after-treatment performance over the broad range of operating conditions which have to be explored for the real driving emissions compliance.

In the first chapter, a brief overview of the phenomena involved in automotive reactors is presented and the fundamental equations used to reproduce such phenomena in the simulations are described.

In the second chapter a 1D-CFD numerical model developed for an innovative Lean NO_x Trap catalyst is presented. The component, optimized for low temperature NO_x storage, was extensively characterized at the Synthetic Gas Bench (SGB) in terms of oxidative behaviour, NO_x storage under fuel-lean conditions, Oxygen Storage Capacity (OSC) and NO_x reduction under alternating fuel-rich and -lean conditions. The experimental results were used to calibrate the LNT model reaction parameters by means of optimization tools based on evolutionary algorithms. The calibrated model was finally validated over different WLTC and RDE driving cycle data to assess its predictive capabilities over transient operating conditions.

In the last chapter, a comprehensive methodology to extensively characterize complex after-treatment systems is presented. The methodology was used to analyze two Euro6-compliant after-treatment architectures for diesel passenger cars, which included a Diesel Oxidation Catalyst (DOC) mounted in closed-coupled con- figuration with an ammonia Selective

Catalytic Reduction (SCR) catalyst coated on a Diesel Particulate Filter (DPF), also known as SCR on Filter (SCRoF or SCRF). First, an experimental campaign was carried out to characterize the analyzed systems in terms of physical and chemical properties of the monoliths, the Urea Water Solution UWS spray characteristics and the NO_x conversion efficiency under type-approval representative operating points. The experiments highlighted a performance gap between the two architectures, especially in the low temperature operating conditions. To further investigate the different systems behaviour and to clarify the source of the performance gap observed in the experimental campaign, a 3D-CFD numerical model was developed for the two systems and used to analyze the internal fluid and thermal dynamics, the UWS spray break-up and evolution, the liquid film development and the flow uniformity at the entrance of the SCRoF catalysts. The numerical analysis demonstrated that the different conversion efficiency achieved by the systems was mainly due to the different architecture of the UWS mixer, providing useful insights for the compact and efficient design of similar after-treatment components.