Study and analysis of Soot Filter Regeneration by using the Lattice Boltzmann Method

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Abstract

The control of the emission of carbon black is an important task in many fields of application, with the transport sector being one of the most important domains. Diesel engines, still being extensively used worldwide, are one of the main contributors to the anthropogenic emission of carbon black. In order to counteract the detrimental effect of carbon black on human health, exhaust gas treatment has been the focal point of research for many decades. State of the art soot filters use a ceramic honey-comb structure, acting as wall flow filters. These filters require periodic regeneration once a critical filter back-pressure is reached. Regeneration is conduced either as active regeneration at elevated temperatures (>600 °C) or continuously, as passive regeneration at temperatures starting from 300 °C. The necessary exhaust gas temperature of active regeneration results in a fuel penalty, making the precise control of the regeneration process imperative. Previous works suggested that the mesoscopic morphology of soot and its evolution during soot combustion influence the reactivity, thus affecting the regeneration process. Hence, the control of the regeneration system requires precise knowledge of the physical and chemical phenomena at hand, necessitating simulations of the regeneration process. In this thesis, a simulation framework to model gas flow, consisting of the different reactive species, taking into account solid-gas interactions, is created. Furthermore, conjugate heat transfer, heterogeneous reactions and the release of reaction heat at the interface between the solid and gas phases is treated. For this purpose, the lattice Boltzmann method (LBM), due to its mesoscopic nature, is chosen as an excellent tool to model the heterogeneous combustion on the pore scale. Within this thesis, a LBM framework is created and appropriate methods to model soot combustion are chosen and extensively validated. A procedure to use focused ion beam scanning electron microscopy (FIB-SEM) data of realistic soot samples for the combustion simulation is implemented. Furthermore, the combustion regimes are analysed based on variation of Péclet number, Damköhler number, and oxygen mass fraction in the inlet gas stream. Simulations with realistic soot geometries are performed and the results are compared with experimental results. It is found that the evolution of the specific reactive surface, as received from LBM simulations, is not comparable to the experimental results. Transmission electron microscopy (TEM) analysis and Raman spectra of the soot before and after combustion experiments revealed that combustion affects the primary particles on the nano-scale. For this reason, a separate model to describe the heterogeneous primary particles and their

combustion was created. Subsequently, first simulations with scale-coupling were conducted, by connecting the mesoscopic LBM simulations with the primary particle design on the nano-scale. It is shown that a more realistic increase in specific surface could be achieved in simulations by coupling the mesoscopic LBM model with a nano-scale primary particle model.