The influence of the boundary conditions on the urea-water solution decomposition in case of Closed Coupled Selective Catalytic Reduction systems performance

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The automotive industry is facing increasingly stringent requirements in aspect of pollutants emission, which is considered as one of the main reasons of global warming and climate changes. The most demanding limits relate to the nitrogen oxides (NO_x) emission for diesel engines. Until now, it has been reduced over 85% and 95%, respectively by the successive European Emission Standards and U.S Emission Standards. What is more, further restrictions are just a matter of time. Hence, there is a high need to gain more knowledge in Computational Fluid Dynamics (CFD) modelling and measurement methodology for exhaust systems investigation purposes.

The most promising method for fulfilling NO_x requirements is the urea-water-solution (UWS) based Selective Catalytic Reduction (SCR). The UWS, containing 32.5% of urea, is injected into the hot gases stream. Subsequently passing through evaporation of water, thermolysis of urea and hydrolysis of cyanic acid, the reducing agent (NH_3) is generated. The benchmark of such solution is the ammonia uniformity index at catalyst intake, however current trend of the SCR systems is heading toward closed coupled solution, what reduces available space for UWS decomposition and products mixing. For keeping high SCR performance, the static devices are installed to generate swirls as well as for spray breaking ups, hence spray-wall interaction could be hardly avoided. During the spray-wall impingement undesired chemical reactions could occur and result in by-products as ammeline, melamine, biuret, cyanuric and solid deposition at least.

Development of the SCR systems is always supported by CFD calculations, especially at the beginning of the process when a lot of concepts need to be investigated before prototyping. Due to complexity of the phenomenon a number of different models such as multiphase flow, porosity, injection, spray-wall interaction, turbulence and chemistry are used. Each of them results in increasing computational time. The point is to find proper calculation methodology to perform it in the possible short time with reliable results.

The main objective of this work is the numerical investigation of urea water solution decomposition in closed coupled SCR solution. In the presented paper the influence of the boundary conditions on generated results is shown. The calculations were conducted for idle, light and medium load conditions corresponding to the operating points of a diesel engine. In order to guarantee geometry independence conclusions two different geometry configurations were taken under consideration. The quantities as UWS decomposition, wall-film deposition and the ammonia uniformity index upstream the catalyst were analyzed in aspect of reaching quasi-static state over the calculation time. All calculations were performed by AVL Fire CFD code.

The results show that depending on the mass flow through the system the different calculation time is needed to obtain desirable data. The NH_3 average uniformity index for low and medium mass load is quasi-stable after 8 UWS injections, whereas for the idle operating point more cycles are needed. There is also distinct dependency between mass load and decomposition rate. Despite the fact that high mass load generates bigger turbulence, the time is too short for evaporation, thus less mass evaporated direct from the spray in behalf of spray-wall interaction. Simultaneously, for low and idle conditions the ratio remains constant.