## **3D SIMULATION OF AN SCR SYSTEM WITH COMPLEX CHEMISTRY IN THE CATALYST**

## Carlo Locci<sup>1</sup>, Karin Fröjd<sup>2</sup>

 Siemens Industry Software GmbH, Nordostpark 3 90403 Nuremberg Germany, carlo.locci@siemens.com <u>Siemens-PLM</u>
Siemens Industry Software AB, Box 14153, SE-400 20 Göteborg, Sweden, karin.frojd@siemens.com <u>Siemens-PLM</u>

SCR is the main technological solution used to abate nitrogen oxidizes (NOx) in Diesel cars. NOx abatement is achieved through a spray of urea, injected in the turbulent exhaust gases flow, that leads to gaseous ammonia production. The reactions of ammonia with NOx are promoted in a catalyst, in which solid/gas heterogeneous reactions occur between the gas and the catalytic metal. Modeling SCR is quite challenging. Accurate turbulence modeling is required to predict the mixing between the gas and the spray. Also, the spray interaction with the wall is quite critical to guess the right temperature at the wall. Finally, complex chemistry at the catalyst is needed to predict the final global amount of NOx downstream the SCR device. In this work, we report the results of a complete SCR setup, with spray, spray-wall interaction and complex chemistry at the catalyst. Turbulence modeling is carried out with Detached Eddy Simulations (DES) and numerical results are compared for the global ammonia over NOx ratio at the catalyst inlet and for the global NOx amount at the catalyst outlet. The mechanism from Olsson et al. [2] is used to simulate the heterogeneous reactions. Experimental results are taken from the work of Abidin et al. [1]. Results are in fair agreement with the experimental data.

## REFERENCES

[1] Z. Abidin et al, 3D-Semi 1D Coupling for a Complete Simulation of an SCR System. *SAE Technical Paper*, Vol. **2013-01-1575**, 2013.

[2] L. Olsson et al, A kinetic model for ammonia selective catalytic reduction over Cu-ZSM-5. *Applied Cat. Env.*, Vol. **81**,2008.