Siemens Digital Industries Software

Improving the air quality in our cities

Reducing airborne pollution with Simcenter STAR-CCM+

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Contents

Introduction

According to the World Health Organization's (WHO) report, "Ambient air pollution: A global assessment of exposure and burden of disease," 3 million deaths globally were attributable to air pollution in 2012 alone, and only 10 percent of the world's population lives in a city that complies with WHO air quality guidelines. A major source of air pollution can be sourced to combustion by-products, which in urban areas and cities is heavily influenced by vehicle emissions.

One approach to reduce the harmful pollutants, specifically nitric oxides, that are emitted from any form of combustion – be it automotive, marine or even in power generation – is the not so commonly known technology of Selective Catalytic Reduction (SCR). SCRs work by introducing a spray of either ammonia, urea or a mixture of urea and water (AdBlue) as a carrier fluid to the exhaust gases in the exhaust system. Once the solution is injected, underlying chemical reactions take over to reduce the harmful polluting nitrogen oxides (NO_x) as it flows through the exhaust system.

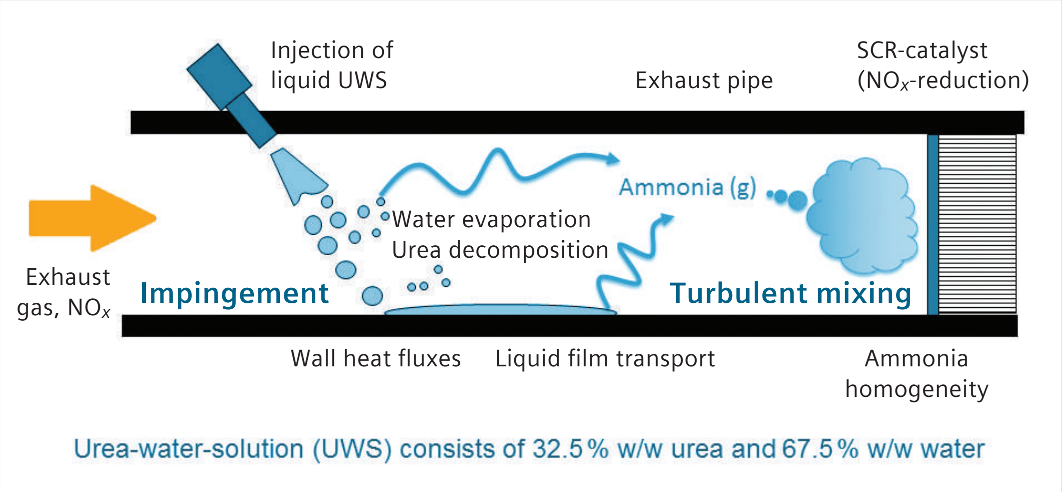


Figure 1: SCR process – solution injection, wall interaction, gas formation and mixing.

How SCRs work

The physical and chemical processes that underpin this technology are highly complex, and despite SCRs being in use for over 60 years, research into the fluid mechanics governing their effective design is ongoing. The research team at the Institute for Powertrain and Automotive Technology at Vienna University of Technology, headed by associate professor Thomas Lauer, has been responsible for a great deal of work in this area. They use a combination of physical experimentation and computational fluid dynamics (CFD) simulation with Simcenter™ STAR-CCM+™ software, the flagship CFD code of Siemens Digital Industries Software.

As Lauer explains, "The AdBlue droplets impinge on the hot surfaces of the exhaust system. Particularly at low system temperatures liquid film is formed. Ammonia gas is then formed by dehydrating the injected solution, which undergoes thermolysis and hydrolysis. Once the ammonia gas is formed, it is mixed with the hot exhaust gas before reaching the catalyst (where the NO_x reduction takes place). So it is necessary to predict turbulent mixing in the pipe to ensure flow uniformity prior to the catalyst." The complete process is shown schematicallyin figure 1.

Another key consideration is the interaction of the droplets from the injected solution and the hot metal surfaces of the exhaust system. As figure 2 shows, the behavior of the droplets and whether or not they rebound, break up or stick to the surface is a function of the droplet Weber number (We) – the ratio of the droplet's inertia to its surface tension – and the wall temperature where it impacts. Due to the work at the Vienna University of Technology, the team adopted a regime boundary between wall wetting and non-wetting that introduced a transition region, between $T_{DL,u}$ and $T_{DL,l}$, as shown in figure 2. The increased understanding of this phenomenon led to a better prediction of the ammonia uniformity, a fundamental index for SCR systems, which quantifies the quality of the mixing between ammonia and the main flow, and is measured prior to the chemical reduction in the catalyzer.

Their cutting-edge work is possible due to a wide range of tools at their disposal. For physical testing, a combination of infrared cameras and thermocouples measure wall temperatures, as well as laser diffraction to document droplet breakup. Ammonia concentrations are derived from the nitric oxide distribution measured by chemi-luminescence detectors (CLD) and Fourier transform infrared (FTIR) spectroscopic gas analyzers.

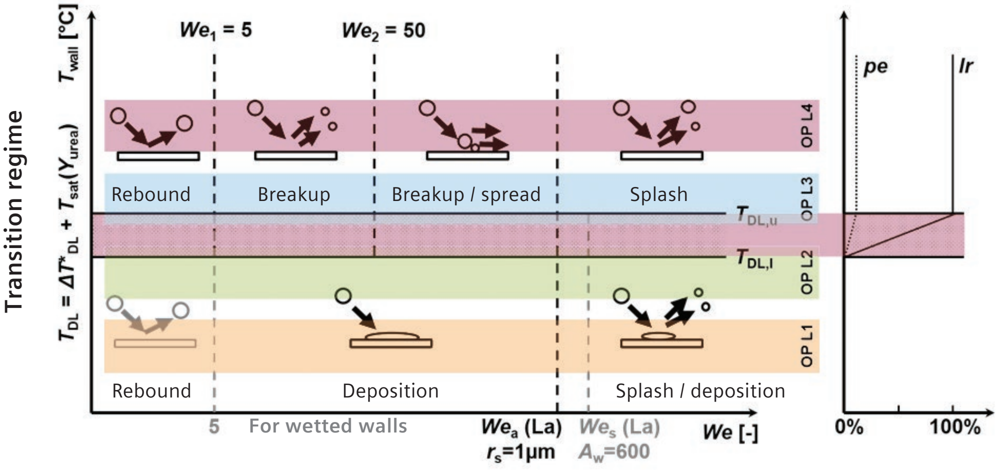


Figure 2: Droplet behavior when interacting with different surface temperatures.

Source: Smith, H., Zöchbauer, M., Lauer, T.: "Advanced Spray Impingement Modelling for an Improved Prediction Accuracy of the Ammonia Homgenisation in SCR Systems." SAE Technical Paper 2015-01-1054, 2015, doi:10.4271/2015-01-1054.

Turbulent mixing

As turbulent mixing is an important physical process in the SCR, its ability to be numerically modeled in CFD was validated against a cold flow exhaust system that was fitted with optical access (see figure 3) to measure the instantaneous velocity field with a laser Doppler anemometry (LDA) system. CFD simulations were then carried out on the exact experimental setup with Reynolds Average Navier Stokes (RANS) and large-eddy simulation (LES) approaches to turbulent modeling.

The time-varying LES simulation calculates the velocity and flow structures typical of transient flow patterns in the mixing pipe. As Lauer points out, “Both the velocity and turbulent fields are important to take convective and diffusive transport into account.” The three cross sections through the exhaust in figure 3 show the Reynolds stress in the main flow direction (uu) for the LES and the LDA compared to the turbulent kinetic energy of the k-ϵ Realizable model. It shows that the two equation turbulence model (RANS) values for turbulence are underpredicted, therefore the higher fidelity LES model is closer to reality (for example, the LDA results).

The reasoning is that RANS models only give a simplified representation of the turbulent kinetic energy field in a complex turbulent flow field, as the turbulence models are typically validated for simple flow patterns. The LES model solves for turbulence that is anisotropic in complex real life flows. The right specification of turbulence is critical as the gas transport in the flow is closely related to the turbulent kinetic energy.

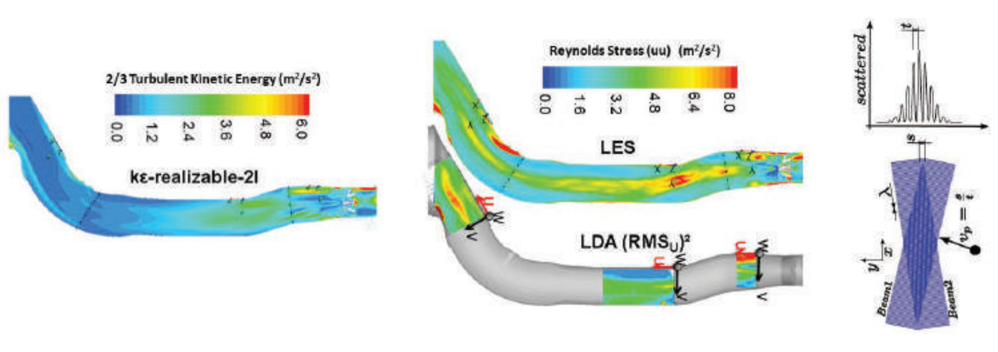


Figure 3: Cold exhaust flow turbulence validation.

The impact of turbulent mixing on ammonia concentration

Two SCRs with swirl mixers were investigated with respect to ammonia distribution at the SCR catalyst, one with a long mixing section and another with a short mixing section and two different mixer blade angles (35 and 45 degrees).

The results for the short mixing section are shown in figure 4 at two operating points. The results for the long mixing section are shown in figure 5 at four operating points. In both cases, the local ammonia concentrations were derived from CLD measurements at 65 positions at the SCR outlet. The experimental results are plotted in both figures as a benchmark for the CFD simulation.

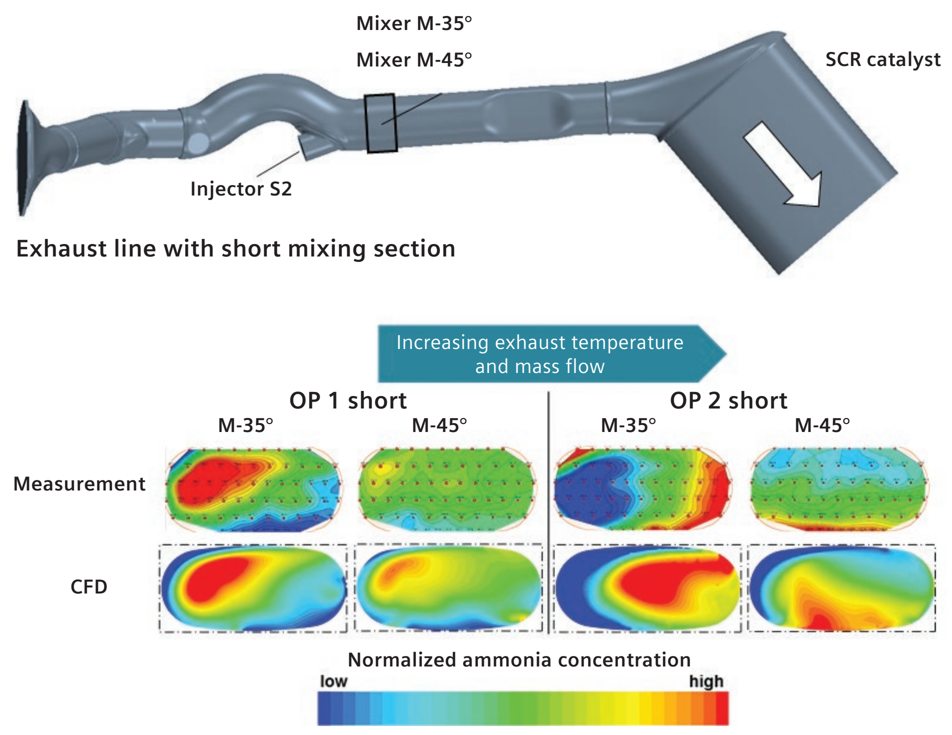


Figure 4: Short pipe ammonia distribution downstream of SCR catalyst.

Source: Zöchbauer, M., Lauer, T., Hofer, G. and Krenn, C.: "CFD-Simulation and Validation of the Ammonia Homgenisation in SCR Systems." 9th International Exhaust Gas and Particulate Emissions Forum, Ludwigsburg, 2016.

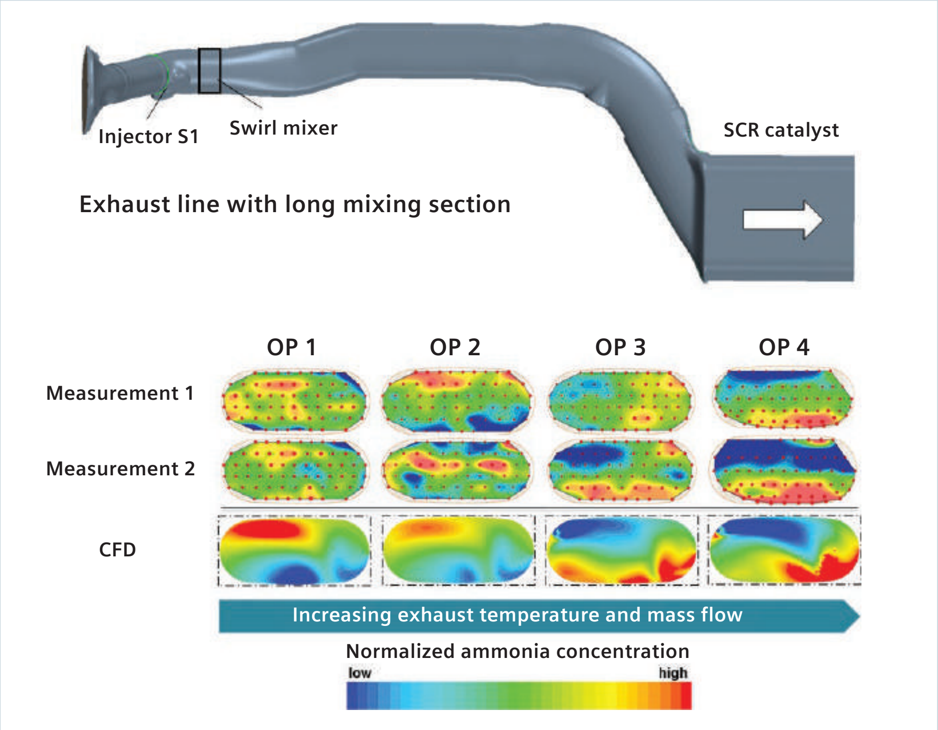


Figure 5: Long pipe ammonia distribution downstream of the SCR catalyst.

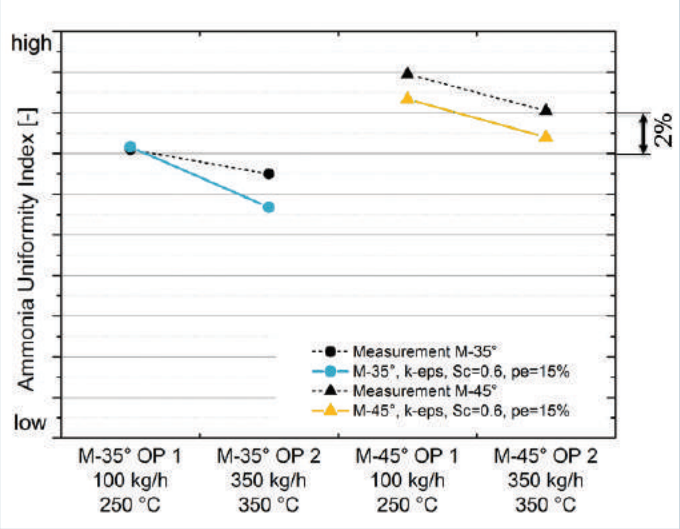


Figure 6: Short pipe ammonia uniformity comparison for 35- and 45-degree mixers.

Generally, a good correlation between the simulation results and the measurements can be observed for both exhaust systems. As expected, the longer mixing section shows better uniformity compared to the shorter mixing section. The region with high ammonia concentration (the hotspot) moving from the upper left to the lower right from OP1 to OP4 can be represented with the CFD simulation, see figure 5.

The tendency of the exhaust system with the short mixing pipe and 45-degree mixer (M-45°) to have better ammonia uniformity at both operating points compared to the concept with the 35-degree mixer (M-35°) was reflected in the CFD simulation, too.

Figure 6 plots the ammonia uniformity index and shows the general trends of the two investigated operating points and the two mixer concepts were well represented by the CFD simulation.

Source: Zöchbauer, M., Lauer, T., Hofer, G. and Krenn, C.: "CFD-Simulation and Validation of the Ammonia Homgenisation in SCR Systems." 9th International Exhaust Gas and Particulate Emissions Forum, Ludwigsburg, 2016.

Risk assessment procedure to determine deposit formation

Deposit formation from the urea-water solution (AdBlue) is a complex process that requires accurate physics modeling when performing numerical simulations of SCRs. The ability to directly simulate the chemical process behind deposit formation and ammonia gas generation is not explicitly modeled or calculated in this study as the time scales are longer than is currently practical for CFD. But Lauer and his team have created an analysis metric of the wall film that is critical to deposit formation. It started with basic experimental measurements to visualize the liquid film behavior prior to deposit formation, namely:

1. For the wall film flowing over a blade, deposition occurs at places where it stagnates
2. Where there is a high supply of liquid urea/AdBlue on a surface, no deposits form
3. If droplets trickle over the trailing edge of surfaces, deposits form downstream

From these observations criteria were derived and implemented in a postprocessing routine to analyze the liquid film with respect to a deposit formation risk; the structure of the routine is shown in figure 7. The methodology was further calibrated against experiments to prove the robustness of the routine and its ability to represent the most critical effects of deposit formation.

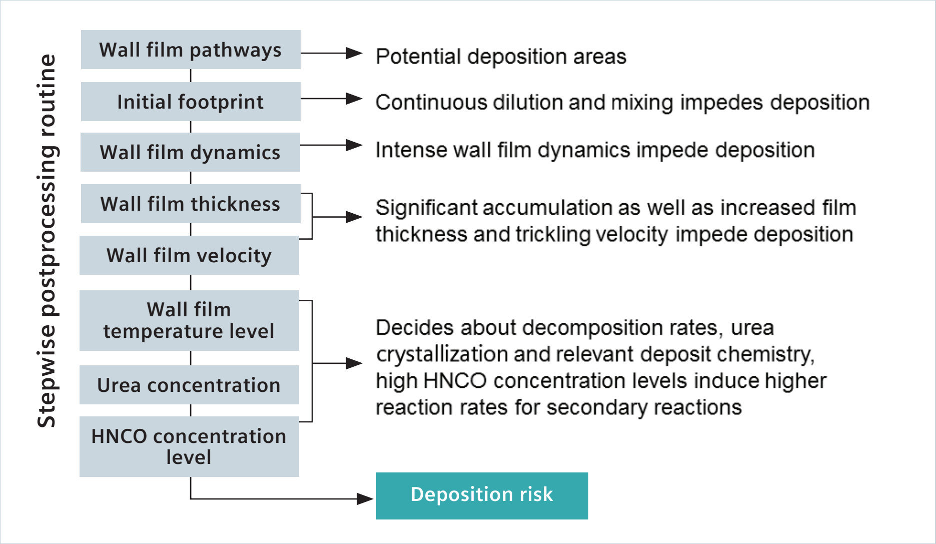
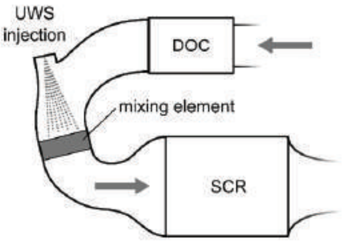


Figure 7: Deposit risk formation flowchart.

Source: Smith, H., Lauer, T. and Pierson,S.: "Optical and Numerical Investigations on the Mechanisms of Deposit Formation in SCR Systems." SAE Int. J. Fuels Lubr. 7(2):525-542, 2014, doi:10.4271/2014-01-1563.

Putting the deposit formation risk postprocessing routine into practice, CFD and experiments were performed on the close-coupled SCR system shown in figure 8. There were two mass-flow rates of urea water solution tested, 35 and 60 milligrams per second (mg/second). The experiment was run for 90 minutes, but for practical reasons the CFD was used to simulate only a few seconds of physical time. The CFD simulation predicts one trailing edge deposit at the left-hand side when looking from the rear for the lower urea solution flow rate. At the higher urea mass flow rate, three rearward blades are predicted to have deposits. Overall, there is very good agreement for the routine for the test case.

Close-coupled SCR system



Investigated operating point:

$T_{exh.}$	[°C]	275
$\dot{m}_{Exh.}$	[kg/h]	175
$\dot{m}_{UWS}$	[mg/s]	35, 60
$f_{inj.}$	[Hz]	3

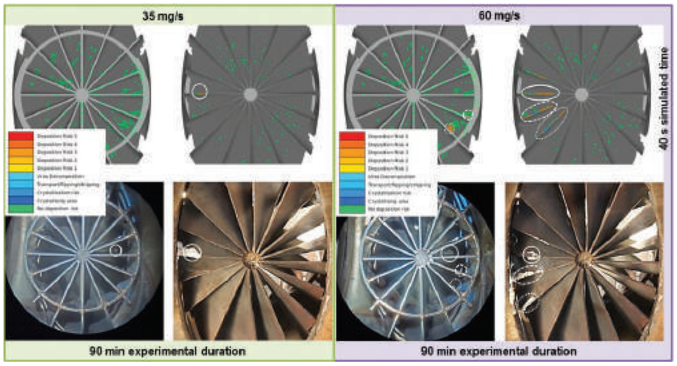


Figure 8: Deposit formation on mixer blade, CFD results on top and experiments on the bottom.

Source: Smith, H., Lauer, T., Schimik,V. and Gabel, K.: "Evaluation and Prediction of Deposit Severity in SCR Systems." *SAE International Journal of Engines* 9(3):1735-1750, 2016, doi:10.4271/2016-01-0970.

Conclusion

The work from the Institute for Powertrain and Automotive Technology at Vienna University of Technology has shown that SCRs, impingement, liquid film formation and turbulent mixing are important to ammonia transport in the system and the choice of turbulent modeling strategy is crucial. The ability to predict turbulence mixing with LES modeling in Simcenter STAR-CCM+ shows that good agreement between CFD and experimental measurement is possible. Additionally, a risk assessment routine was developed by the team at Vienna University of Technology based on experiments in order to evaluate deposit formation of the urea-water solution.

This highlights the ability of CFD, when it has been expertly calibrated against physical experimentation (whether from literature or own experiments), to predict trends and performance. This allows many more design iterations to be carried out so there is confidence that once a testing prototype is manufactured, it will perform as expected. This not only saves the manufacturer time and money but improves the air quality in our cities and contributes to our health.

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