

Impact of the Turbulence Model and Numerical Approach on the Prediction of the Ammonia Homogenization in an Automotive SCR System

Simon Fischer, Rene Bitto and Thomas Lauer
Vienna University of Technology

Christian Krenn, Johannes Tauer and Guenther Pessl
BMW Motoren GmbH Steyr

ABSTRACT

The Selective Catalytic Reduction (SCR) is a promising approach to meet future legislation regarding the nitric oxide emissions of Diesel engines. In automotive applications a liquid urea-water-solution (UWS) is injected into the hot exhaust gas. It evaporates and decomposes to ammonia vapor acting as the reducing agent. Significant criteria for an efficient SCR-system are a fast mixture preparation of the UWS and a high ammonia uniformity at the SCR-catalyst. Multiphase CFD-simulation is capable to support the development of this process. However, major challenges are the correct description of the liquid phase behavior and the simulation of the ammonia vapor mixing in the turbulent exhaust gas upstream of the SCR-catalyst.

This paper presents a systematic study of the impact of the turbulence model and the numerical spatial discretisation scheme on the prediction of the turbulent mixing process of the gaseous ammonia. The simulations are carried out for an exhaust system with a mixing element that creates turbulent swirl flow in the mixing pipe. Numerical results are validated with back pressure measurements at the mixer and CLD-measurements of the spatial distribution of the reduced NO_x -concentration at the catalyst outlet.

The study proves the high impact of an advanced second order differencing scheme on the species transport. Furthermore it shows that Reynolds-averaged k- ϵ -models systematically underestimate the turbulence level in the swirl flow and, in consequence, the turbulent diffusion and uniformity of the ammonia vapor at the catalyst. In contrast, a Reynolds-Stress-model leads to improved predictions by accounting for the anisotropic character of turbulence in the swirl flow. In combination with detailed sub models of the liquid phase dynamics and -evaporation a correct prediction of the ammonia homogenization for a wide range of operating conditions can be achieved. By this means a good correlation with measured ammonia uniformity indices and the mixing element's back pressure behavior can be observed. The described numerical method therefore allows for a predictive evaluation and optimization of SCR-mixing systems.

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INTRODUCTION

Legislative restrictions are forcing the automotive industry to further reduce nitrogen oxide emissions of Diesel engines significantly [1]. As engine modifications have reached their limits to fulfill the EURO VI or the US TIER 2 BIN 5 regulation with reasonable effort, exhaust gas aftertreatment has become a necessity [2]. In the sector of midsized and big passenger cars, the Selective Catalytic Reduction with ammonia as a reducing agent is considered as

a promising technical solution to cope with this challenge and first systems are already on duty [3]. In mobile applications, the technology is based on the injection of a liquid urea-water-solution into the exhaust system. In the hot exhaust the water evaporates and the remaining urea decomposes to ammonia. Ammonia vapor is then used as the reducing agent for nitrogen oxides in a catalytic converter, located downstream of the injection position. Main criteria for the efficiency of the process are a fast formation of the reductant from the UWS and a satisfactory mixing of gaseous ammonia



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with the exhaust, resulting in a uniform ammonia loading of the catalyst under all engine operating conditions. Only if those criteria are fulfilled, a sufficient reduction of NO_x -emissions can be achieved with minimum UWS-consumption and without ammonia slip into the atmosphere [4]. In passenger car applications, the problem is even more pronounced due to the stringent packaging limitations, leading to short preparation and mixing pipes [5]. Therefore, to meet these challenges, a carefully designed mixing section is an imperative.

Multiphase CFD-simulation is in principle capable to support the development of efficient SCR systems. However, major challenges are the correct description of spray dynamics and chemo-physical decomposition of the UWS, as well as the simulation of ammonia vapor mixing in the turbulent exhaust gas upstream of the SCR-catalyst.

A lot of efforts have been made to model and validate the decomposition process of the UWS, e.g. [6, 7]. Moreover, droplet dynamics in the turbulent flow field have been studied in detail [8] and models for simulating the droplet wall-interaction have been proposed [9, 10] and adapted to SCR-CFD-simulation [11, 12]. Nevertheless, most of the CFD-studies in literature have not focused on the relevance of turbulence modeling when predicting the ammonia homogenization. All of the so far published numerical studies have applied a two-equation (k - ϵ -) RANS-model for the exhaust gas flow. Moreover, a direct comparison between numerically predicted and measured uniformity can merely be found. A detailed literature review will be given in the following sections. Interestingly, all of the cases that have been validated regarding homogenization [13, 14] - including previous works from the authors [12, 15] - underestimate the measured ammonia uniformity to some extent.

For this reason, this paper presents a systematic study on the impact of the turbulence model and numerical differencing scheme on the prediction of the turbulent mixing process of gaseous ammonia. The study is carried out on a production type passenger car SCR-exhaust system, including a swirl mixer, see section 3. The model setup with particular emphasis on turbulence modeling, scalar mixing and numerics is described in section 4. Numerical results are validated with back pressure measurements of the system and CLD-measurements of the spatial distribution of the NO_x -concentration at the catalyst outlet (see sections 5 and 6).

REVIEW OF TURBULENCE- AND AMMONIA MIXING- MODELS IN SCR-CFD

Some publications have already described the CFD-simulation of ammonia vapor homogenization and its validation. In any case, ammonia vapor is modeled as a scalar released from UWS droplets, whose dynamics are described in a Lagrangian approach [16]. The gas flow is always

modeled in an Euler description. Two way coupling is taken into account.

Bhattacharjee et. al. [17] conduct sensitivity studies regarding several sub processes of UWS preparation and ammonia homogenization. However, in any case the turbulence is modeled by a standard k - ϵ -high Re model with wall functions. Simulating ammonia homogenization, the authors conduct a sensitivity study on mesh resolution in a straight pipe geometry. They state that differences of ammonia concentrations predominantly appear in the near wall region. The effect is described to be extremely small for intermediate and fine meshes (cell edge sizes 10 mm, 5 mm) and only relevant for a very coarse mesh (20 mm). In a more complex geometry they analyze the sensitivity of ammonia mixing to the porosity index, for the widely used porous medium approach for the SCR brick. Major result is that the effect is very small, concluding that any resistance different from zero will be adequate to leave homogenization predictions unchanged. In a further study they compare the basic straight pipe to a modified straight pipe configuration with a 90°-bend upstream of the injector. The modification leads to a distinct swirl flow downstream of the injection. The velocities, normal to the main flow, are comparable to the axial ones. As a consequence, ammonia homogeneity at the catalyst intake is significantly enhanced. A quantification of the effect is not presented. Finally, the authors describe the experimental validation of the ammonia homogenization prediction for a heavy duty vehicle SCR system. The proposed model covers general trends in the ammonia distribution at the catalyst inlet correctly. A quantitative comparison is regarded as difficult and not conducted, due to the limited number of measurement spots.

Another work offering some validation data regarding ammonia homogenization is published by Birkhold [13]. The author simulates the homogenization of ammonia in a straight pipe setup, with a 45° spray injection angle relative to the main flow direction, targeting on the opposite wall. UWS decomposition is described by evaporation laws. The released ammonia scalar is transported in the turbulent flow field, simulated with a standard k - ϵ -high Re model. The predicted ammonia distribution at the downstream catalyst is compared to concentration measurements at nine discrete spots for two engine operating conditions. The agreement is described as sufficient, with a good correlation of ammonia maxima locations. Nevertheless, Birkhold describes significant quantitative deviations in the predicted reductant distributions, without quantifying them. From the distribution figures, an overestimation of simulated concentration gradients in the catalyst intake plane can be observed. As a probable explanation the author takes the neglecting of real pipe features, like welded seams and small kerbs, into account. Regarding model insufficiencies, he considers the impingement model as an error source.

Gehrlein et. al. [14] compare different mixing elements and a no-mixer setup in a straight pipe with respect to back pressure and uniformity of ammonia. Though their

publication focuses on experimental data and methodology, they shortly describe a CFD-model and a validation case. Again, a standard k- ϵ -high Re model is used [18]. For the validated mixer case, the simulation yields a UI of 0.90 at the catalyst, in comparison to a measured value of 0.93. The simulated ammonia distribution is qualitatively correct, but reveals steeper gradients from rich to lean ammonia regions.

The authors of the paper at hand have previously also published a CFD-model of the UWS preparation and ammonia homogenization, validated with data from the engine test bench [12]. The analyzed, simplified SCR system consists of an s-bend leading into a straight pipe with a recessed injector, targeting on the opposite pipe wall in 45° to the main flow. Like in the setup of Birkhold, spray wall-interaction is provoked for impingement model validation purposes. The model includes an Euler-Lagrange description of the two phases, with a standard k- ϵ -high Re model for the exhaust flow. Phase transition from liquid urea to ammonia is modeled with an evaporation approach leading into an ammonia scalar. All transport equations are solved with a second order differencing scheme (MARS). Though the model shows a good correlation with experiments regarding the liquid phase, it systematically underestimates the ammonia uniformity at the pipe outlet, measured by FTIR, for all analyzed operating conditions. The same trend has been observed, when employing the model to a production type passenger car SCR-system including a swirl mixer [15]. Again, an overestimation of gradients in the simulated ammonia distribution and an underestimation of the predicted uniformity have been noticed.

Further publications are limited to numerical sensitivity studies without offering validation data:

Jeong et. al. [19] analyze the relevance of UWS injector position, -hole number and -pressure on the ammonia uniformity at the SCR catalyst with the CFD method. They employ a k- ϵ -RNG turbulence model with a second order differencing scheme (MARS) for the gas phase flow. A major result is that increasing the distance between injector and catalyst leads to a rise of the ammonia uniformity index.

Yi [20] analyzes the effect of two different mixers on the homogenization. Like Jeong et. al. he uses a k- ϵ -RNG model for turbulence. The geometry consists of a straight pipe, leading into the catalyst inlet cone under a small angle. The UWS injector is located at the pipe wall in some distance upstream of the catalyst, releasing the UWS spray in a 45° angle relative to the main flow. Without a mixer, poor uniformity of ammonia at the catalyst inlet face is observed. Integrating a helix swirl mixer leads to a rise of uniformity, a small plate mixer (no swirl) produces a less improved UI.

In a very similar manner, Zhang et. al. [21] numerically analyze the impact of a static mixing element on the ammonia homogenization in a straight pipe exhaust systems. They vary the mixer position relative to the injector, mixer blade number, -shape and blade twisting angle. In contrast to all other works cited here, they use a simplified gaseous ammonia injection. The turbulent flow is described by a

standard k- ϵ -model. For the straight blade mixer, the major enhancement in ammonia uniformity is predicted within a very short distance. With a twisted blade mixer the effect on mixing of ammonia is observed to last further downstream, but to be less intense on a short scale. The observation is in agreement with Yi's results [19]. The authors explain the simulated behavior as a result of a trade-off between small scale turbulence and large scale swirl.

Krenn et. al. [22] describe a CFD simulation for a passenger car SCR system, with the UWS spray injector targeting on an integrated blade mixer. Urea decomposition is simulated with an evaporation approach, and ammonia vapor treated as an active scalar. Turbulence is modeled with k- ϵ -RNG. For transport equations of turbulence and scalars a first order upwind scheme is used, while momentum is discretized with a second order scheme. The authors optimize the mixers rotational position, in order to maximize the UI at the catalyst.

REVIEW OF TURBULENT FLOW MODELING AND SCALAR MIXING

To understand the systematic underestimation of ammonia homogenization, observed in any validated SCR system simulation, a closer look to the theory of scalar mixing and turbulence modeling is necessary.

An interesting statement on the relevance of turbulence models in SCR systems is published by Ström et. al. [8]. Though the authors focus on the dynamics of UWS droplets, they point out a fact that might as well be relevant for the scalar phase in the turbulent exhaust flow. Analyzing relevant forces for a precise CFD model of droplet dynamics in an Euler-Lagrange approach, they find the turbulent dispersion to be one of the most crucial effects. However, the authors state that the outcome of the turbulent dispersion model is directly linked to the quality of the turbulence model's predictions. They notice that a k- ϵ -RNG model, which they employed throughout their study, might in that sense be critical, due to its inherent limitations. The main drawback of the model is, according to Ström et. al., its isotropic turbulence assumption, i.e. an equality of all coordinate directions with respect to turbulent velocity fluctuation. They conclude that a more advanced turbulence model might be necessary, especially when analyzing more complex geometries including bends, diffusers, etc.

A very similar statement can be found in an early work on turbulence models by El-Tahry [23]. He compares the results of a standard k- ϵ -model, a simplified constant diffusivity model and the more sophisticated Reynolds stress model (RSM) to velocity measurements in an engine-like geometry. The main finding is that both, the k- ϵ - and the RSM, cover the mean velocities in good agreement. However, only the RSM with its tensor character is able to predict realistic levels of anisotropy of turbulence components, in direction normal to the main flow. The two equation model was proved to be incapable of such calculations. El-Tahry underlines that this

difference is especially pronounced, if strong normal stresses occur, e.g. in swirl flows. The author states that this might become especially important considering scalar diffusion.

Tominaga et. al. [24] review a number of CFD works on the diffusion of scalars in different types of turbulent flows, modeled by RANS equations. The reviewed cases include a scalar jet injection into a crossing flow and the dispersion of a plume from a single point source in an open field environment and around buildings. All cited studies undertake an adaption of the turbulent Schmidt number to better match the scalar's measured concentration distributions. This adaption can - according to the authors - be regarded as a compensation of underestimated turbulent momentum diffusion, i.e. underestimated turbulent viscosities, by the turbulence models. This can be seen from the theoretical Schmidt number introduction: All k- ϵ -turbulence models are based on the eddy viscosity hypothesis [16]. To model momentum coupling of neighboring flow sections by small scale vortices, the turbulent viscosity μ_t is introduced and related to the turbulent kinetic energy k and dissipation ϵ :

$$\mu_t \sim \frac{k^2}{\epsilon} \quad (1)$$

With regards to scalar transport, a direct proportionality of turbulent diffusive momentum- and scalar transfer between sheering flow layers is assumed. This means, the turbulent scalar diffusion, l.h.s. of equation (2), is directly linked to the turbulence model's viscosity prediction:

$$\rho \overline{u_j' Y'} = - \frac{\mu_t}{Sc_t} \frac{\partial Y}{\partial x_j} \quad (2)$$

The constant of proportionality Sc_t is the turbulent Schmidt number. An underestimated turbulent viscosity must therefore be compensated by reducing the Schmidt number from its standard value (0.7 - 0.9).

The publication at hand therefore identifies an adequate description of turbulence, for an efficient but precise modeling of ammonia mixing in typical SCR exhaust systems.

GEOMETRIC SETUP AND OPERATING CONDITIONS

Figure 1 shows a sketch of the SCR system geometry that has been used throughout the study. The system can be regarded as a state-of-the-art passenger car SCR mixing section, such, that the following results claim to be of general interest for the simulation of typical UWS based SCR systems. The analyzed CFD domain covers the exhaust line from downstream the DPF to the outlet pipe of the SCR catalyst. This includes the UWS injector location, which is integrated into a pipe bend to realize a tangential injection of the UWS spray. The spray cone from a three hole nozzle

(SMD 140 microns) is directly targeted onto the center of a static swirl mixer (see close up in Figure 1). The following mixing section changes from circular to an oval/flat cross section for packaging reasons and leads - after a bend - smoothly into the SCR catalyst. The mixing length from mixer to catalyst inlet is approximately 950 mm.

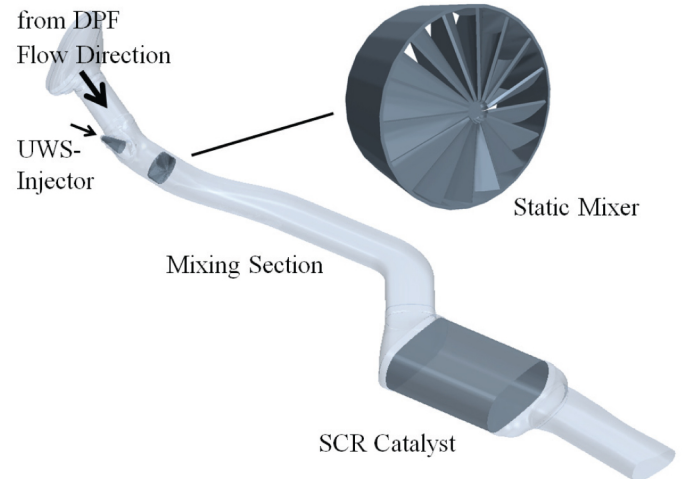


Figure 1. Exhaust system geometry at SCR-Mixing-Section

The CFD mesh consists of approximately 2.1 Mio. computational cells, including about 0.4 Mio solid cells for the mixer and pipe walls, to correctly model their thermal behavior with conjugate heat transfer (CHT) [12]. The SCR catalyst is modeled with a structured hexahedral mesh to apply a porous medium description [17]. The remaining geometry is meshed with polyhedral cells. No mesh independence study is conducted. Instead, the cell base size is chosen at a size of approximately 3 mm, which leads to a cell count typical for an industrial development process. The base grid size is in accordance to the findings by Bhattacharjee et. al. regarding mesh insensitivity [17]. Local refinements are undertaken in the mixer region. An extrusion layer covers the near wall regions throughout the geometry, to allow a correct simulation of the turbulent boundary layer.

The analyzed operating conditions are summarized in Table 1. Each operating point is characterized by an exhaust gas mass flow and temperature, as well as by a NO_x engine raw emission, that determines the UWS injection strategy.

Table 1. Analyzed operating conditions (OP 1, used for sensitivity studies, marked bold)

Operating Point	0	1	2
Exhaust Mass Flow [kg/h]	75	130	200
Exhaust Temperature [K]	473	523	623
UWS Injection Flow [g/h]	20	43.2	90
UWS Inj. Frequency [Hz]	1.1	2.6	3.0

The selected OPs are considered as representative for typical test cycle conditions, covering a wide range of

exhaust gas flow and temperature. At the engine test bench the conditions are realized by adapting load and engine speed, in the simulation the mass flow (i.e. inlet velocity) and exhaust temperature are implemented as an inlet boundary condition.

All sensitivity studies on the turbulence model and numerics are carried out for OP 1. The gained optimum model is applied to all operating conditions. The reason for the choice of OP 1 is explained in the ammonia homogenization results section.

MODEL DESCRIPTION

All simulations are carried out with the commercial CFD code Star-CD [26, 27]. Each simulation set consists of a steady state calculation of the stationary flow field and a transient simulation of the OP including the UWS injection. The former solution is used as an initialization of the latter. Convergence is reached after approximately 1000 time steps for the steady state case.

LIQUID PHASE AND EVAPORATION OF UWS, SOLID MODELING

The UWS spray behavior in the exhaust gas is modeled in an Euler-Lagrange approach with two way coupling [26]. In accordance to Ström et. al. the model accounts for gravity effects on trajectories and turbulent dispersion of droplets [8]. Droplet wall-interaction is modeled by the multi regime Bai-model [9] that has been adapted to UWS behavior [12, 28]. A two dimensional, finite volume liquid film model is included, with shear and gravity effects on film movement [25]. Liquid film's thermodynamic behavior is covered by the Nukiyama pool boiling model [29, 30, 31]. To solve for cooling effects, solid material simulations for pipes and the mixer are conducted with CHT [12]. Outer wall boundaries are modeled with a free convection heat transfer coefficient and constant ambient temperature [22]. Spray boundary conditions are implemented in a user subroutine with the droplet size distribution gained from laser diffraction measurements. The initial UWS temperature is taken from [24].

The UWS is described as a two component fluid with an evaporation approach for both water and urea, considering Raoult's law and boiling [12, 26, 33, 34]. Thermodynamic properties of the two liquid components are taken from literature, according to Birkhold [13]. The saturation pressure curve for urea is taken from Birkhold's latest setup [13] (mind the different proposals by the author made in [11] and [13]). No assumption is made for the water content to define the onset of urea thermolysis, i.e. the model is predictive with respect to the transition from water evaporation to urea decomposition. Melting, evaporation and thermolysis of urea is modeled as a single step process, considering an instantaneous dissociation of gaseous urea in the liquid-gas boundary layer [13, 22]. Therefore, the thermolysis enthalpy is lumped together with melting and evaporation enthalpies

and affecting the droplet/liquid film energy balance [13]. The decomposition of UWS leads to active scalars for water and an ammonia vapor representative. Isocyanic acid is not modeled explicitly. The hydrolysis reaction and further gas phase chemistry is also ignored during simulation. This procedure is based on the assumption that the transport of ammonia and isocyanic acid in the turbulent flow can be regarded as identical, so that the former is representative for both and the latter has not to be considered explicitly. Local FTIR concentration measurements of both species from an earlier research project approve the validity of this assumption [28]. The actual conversion of isocyanic acid to ammonia is therefore considered in the post processing routines only, assuming a very fast hydrolysis at the catalyst.

Water vapor is considered as part of the engine exhaust and therefore of the inlet flow to the CFD domain. Concentrations are gained from FTIR-measurements. The exhaust gas is represented by hot air with temperature dependent fluid properties [35]. Though no chemistry is currently considered in the catalyst brick due to the long time scales of catalyst steady state operation, it is taken into account as a porous medium [17]. This allows for the consideration of brick effects on the upwind flow- and temperature distribution (see e.g. [17]). Though more computational costs arise from this approach, it shifts the specification of outlet boundary conditions from the point of interest at the catalyst inlet plane to a less critical location further downstream.

TURBULENCE AND NUMERICAL DIFFERENCING SCHEMES

Table 2 gives an overview on the model setups that have been analyzed, to identify the impacts of turbulence model and differencing scheme on ammonia mixing. The employed turbulence models are restricted to RANS formulations. The use of a LES- or even DNS model can currently not be regarded as suitable for the computer aided design of SCR systems, due to their computational effort.

Table 2. Analyzed turbulence models and numerical differencing schemes for spatial discretisation

Setup	Turbulence Model	Differencing Scheme (Momentum, Pressure, Turbulence, Scalars)
1	k-ε-RNG [26]	UD (1 st order)
2	k-ε-high Re [26]	UD (1 st order)
3	k-ε-RNG	MARS (2 nd order)
4	k-ε-high Re	MARS (2 nd order)
5	RSM-Speziale [26]	MARS (2 nd order)

From the chosen models, only the RSM accounts for anisotropy in velocity fluctuations that can be found between the main flow direction and normal directions in a turbulent field. As a consequence, the RSM is expected to be more expensive, but also more precise, especially in the expected