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Supporting Information available online

Urea Conversion for Low-Temperature Selective Catalytic Reduction in a Swirled Diesel Exhaust Gas Configuration

A novel design of an AdBlue mixing unit to reduce urea deposits at low temperatures in diesel exhaust is described. The main principle of the mixer includes the injection of AdBlue in an axisymmetric swirling flow, which is achieved by splitting the exhaust stream and off-centred introduction of the sub-flows. Crucial geometric parameters were analyzed by computational fluid dynamics (CFD) simulations towards pressure loss, flow field, and spray morphology. Deposit formation was experimentally investigated on three upscaling levels implying an optical test bench, a diesel engine test bench, and a hydraulic excavator. In particular, the studies with the hydraulic excavator showed neither deposits nor critical back pressure. Overall, the experiments substantiated the working principle of the AdBlue mixer.

Keywords: AdBlue mixing unit, Diesel exhaust, Selective catalytic reduction, Swirling flow, Urea deposits

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1 Introduction

Greenhouse gases (GHGs) are recognized with great concern due to their impact on global warming. Among the GHGs, carbon dioxide (CO_2) is by far the most important one originated from combustion of fossil fuels. Worldwide, many legislative measures have been taken in the past years to reduce GHG emissions. For instance, the European Union (EU) has introduced the Renewable Energy Directive (RED II), which demands a target of 32 % for renewable energy sources by 2030. Also, RED II forces fuel suppliers to realize a renewable energy rate of 14 % for road and rail transport.

In Germany, the "Climate Protection Plan 2050" follows a long-term strategy to reach GHG neutrality. As a consequence, sustainable power train technologies are globally pushed towards electrical drives, fuel cells, and synthetic fuels obtained from renewable sources. A quite rapid implementation of the climate targets can particularly be achieved by an intensified admixture of CO_2-neutral fuel components like biomethane, bioethanol, fatty acid esters or hydrogenated vegetable oil. For such a transitional period, diesel engines with direct injection (DI) might have special attention associated with their high efficiency and low fuel consumption. Due to this efficiency, DI diesel engines are widely established for many stationary and mobile applications ranging from vehicles, crafts, and locomotives to work machines, emergency generators, and combined heat and power plants.

However, the combustion of diesel fuel also causes the output of pollutants such as nitrogen oxides (NO_x), hydrocarbons (HCs), carbon monoxide (CO), and particulate matter (PM). Therefore, legislative emission standards have been introduced and tightened demanding efficient abatement measures [1]. For the diminution of CO and HC, diesel oxidation catalysts (DOC) are applied, whereas PM is removed by using diesel particulate filters (DPFs). Furthermore, NO_x are diminished by selective catalytic reduction (SCR), while in passenger cars NO_x storage reduction catalysts are also employed.

The SCR procedure was originally developed for waste incineration plants and implies the reduction of NO_x by ammonia (NH_3) to yield N_2 and H_2O [2]. Typical SCR catalysts are $V_2O_5/WO_3/TiO_2$ (VWT) and Fe- or Cu-containing zeolites. VWT catalysts are mostly used in heavy-duty diesel engines and stationary applications, while zeolites are primarily taken

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for passenger cars related to their activity at low exhaust temperatures as well as stability at elevated temperatures.

Due to its toxicity and hazardousness, the ammonia, required for SCR, is produced on board of vehicles from AdBlue, which is an eutectic aqueous solution containing 32.5 wt % urea ($CO(NH_2)_2$). AdBlue is stored in a separate tank and is injected into the exhaust pipe, where urea is converted according to the overall reaction $CO(NH_2)_2 + H_2O \rightarrow 2NH_3 + CO_2$ [1, 2]. However, the urea conversion is a highly demanding process implying an intricate sequence of sub-steps, of which anyone can form unwanted deposits [3, 4]. Initially, the water of the AdBlue droplets is evaporated in the exhaust line leaving solid urea, which subsequently begins to melt at 132.5 °C. Then, the molten urea is decomposed yielding isocyanic acid (HNCO) and NH_3 ($CO(NH_2)_2 \rightarrow NH_3 + HNCO$). In the last step, the produced HNCO undergoes hydrolysis resulting in the formation of NH_3 and CO_2 ($HNCO + H_2O \rightarrow NH_3 + CO_2$) [5].

The appearance of deposits can occur by inhomogeneities of the AdBlue spray, heat loss during water evaporation, and contact of AdBlue droplets with cold parts of the exhaust pipe. The latter effect often provokes a liquid film, in which urea precipitates and reacts with HNCO to solid biuret ($CO(NH_2)_2 + HNCO \rightarrow C_2H_5N_3O_2$). Additionally, the formed biuret can undergo a follow-up reaction with another HNCO forming cyanuric acid ($C_2H_5N_3O_2 + HNCO \rightarrow C_3H_3N_3O_3 + NH_3$) [6]. As these by-products decompose only above 180 °C (biuret) and 300 °C (cyanuric acid), respectively, they can accumulate in the exhaust line potentially causing back pressure effects. Furthermore, the deposits can cover the SCR catalyst leading to its mechanical deactivation.

Since these effects limit the efficiency of the SCR process, particularly below approx. 220 °C [7, 8], strategies were developed to prevent deposits. For the conversion of urea and hydrolysis of HNCO, different catalysts were investigated, whereas anatase-type TiO_2 was found to be most efficient [9]. Hence, it was claimed that a TiO_2 coating of the interior exhaust pipe enhances the decomposition of urea [10]. However, it was also shown that even with TiO_2 catalysts the conversion of urea remains incomplete and non-selective below approx. 200 °C [11].

Furthermore, Cu zeolite SCR catalysts were recently reported to reveal substantial urea conversion activity in heavy-duty diesel engine exhaust already above approx. 195 °C, whereas VWT is less active [12]. It was also indicated that between 150 °C and 170 °C the reaction of molten urea, existing in bare form or deposited on SCR catalysts, can be limited by mass transport of the water needed. Consequently, biuret is formed as by-product [13].

Another strategy to eliminate deposits is the electrical heating and insulation of the exhaust pipe downstream to the AdBlue dosing inlet [14]. Furthermore, static mixers located between AdBlue injection unit and SCR catalyst are currently used. These mixers provide hot surfaces and therefore suppress cooling effects as well as wall wetting. Moreover, the mixers provoke turbulences leading to enhanced distribution of the AdBlue droplets assuring NH_3 uniformity, which is crucial for high SCR efficiency [15].

A review on the state-of-the art of modeling of AdBlue spray, impingement, wall wetting, and deposit formation in mixers was recently published [16]. Additionally, it should be mentioned that starting from original impact mixers more advanced types such as in-pipe swirl mixers and body swirl mixers were increasingly engineered for various exhaust pipe geometries depending on dosing strategies and specific vehicle requirements [17–19]. Exemplarily, a mixing unit with an interior swirl formation was suggested. In this configuration, the exhaust flow is directed by a baffle to an interior tube, which contains apertures forcing the exhaust to flow through them producing strong vortex structures [20].

Furthermore, a design characterized by a swirling flow was proposed by the authors, where the vortex structures are generated through splitting the exhaust gas stream into two parts and directing them into the mixing chamber [21]. This working principle was validated by means of computational fluid dynamics (CFD) simulations and experiments on laboratory scale and an engine test bench under stationary operation conditions, enhancing the distribution of the AdBlue droplets and reducing the formation of deposits. However, potential pressure loss and a further reduction of deposits give rise to a more detailed analysis and an optimization of this setup. Furthermore, the scale-up towards a real engine application has not yet been evaluated so far.

In the present study, the global flow and spray dynamics of the novel AdBlue mixing unit, suggested as a first approach recently [21], were improved by using CFD simulations to decrease its back pressure and to avoid urea deposits at low diesel exhaust temperatures. The formation of deposits was experimentally investigated with the advanced mixing unit by using different setups with varying length scales and complexity. These setups included an optically accessible configuration on the laboratory scale using synthetic exhaust, an exhaust line of a stationary one-cylinder diesel engine test bench, and finally a mobile hydraulic excavator.

2 Design of the AdBlue Mixing Unit

The novel mixing unit investigated in this work was designed to assure a uniform distribution of the AdBlue droplets and NH_3 (spray symmetry), to avoid the formation of deposits and to minimize back pressure effects. Since deposits are mainly formed when the spray droplets come in contact with rather cold parts of the exhaust line [16], the concept of the mixer includes the suppression of the mass flow originated from the AdBlue injector towards the walls of the assembly. The configuration of the novel mixing unit is shown in Fig. 1; numbers denote the exhaust gas inlets (1.1 and 1.2), the gas inlet of the used two-component AdBlue injector (2) and the outlet of the mixing unit (3). Additionally, the diameter of the injector mounting and the mixing unit, d_i[1)] and d_o, as well as the diameter and the angle of the exhaust gas inlets (d_{in} and α) are marked.

The configuration is characterized by a concentric mounting of the injector (2) with respect to the mixing unit (straight pipe). Note, that the SCR catalyst is located downstream of the configuration's outlet. The exhaust gas supply is designed

1) List of symbols at the end of the paper.

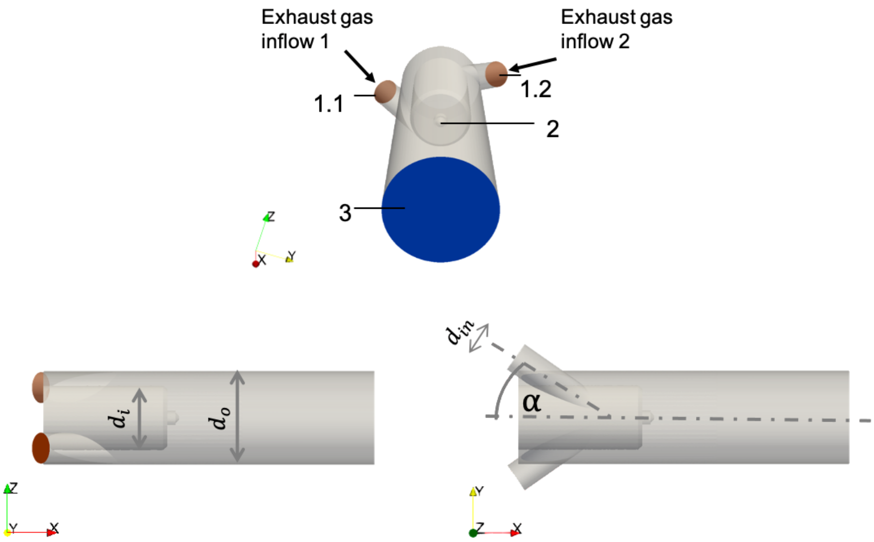

Figure 1. Setup of the novel AdBlue mixing unit. Numbers denote the exhaust gas inlets (1.1 and 1.2), the gas inlet of the two-component injector (2), and the outlet of the mixing unit (3).

having the AdBlue spray dynamics and the pressure loss in mind. Therefore, the exhaust gas stream is split into two streams prior the mixing unit (not shown here) carrying the same mass flow rate, which are supplied by the inlets 1.1 and 1.2 to the mixing unit. Here, the axis of the pipe connected with inlet 1.1 is shifted in negative z-direction, while the axis of the pipe connected to inlet 1.2 is shifted in positive z-direction (related to the coordinate system shown in Fig. 1). This off-centering of the exhaust gas inlets is chosen to introduce an angular momentum of the flow with respect to the injector axis in the annular part of the mixing unit between the injector mounting and the outer walls. With that, a swirl evolves downstream of the injector.

Based on this configuration, two features were identified to influence the pressure drop over the mixing unit, the angle of the inlet pipes relative to the injector axis denoted by α (Fig. 1), and the area ratio A_r. The latter one is defined as:

$$A_r = \frac{A_{mix}}{A_{in}} = \frac{d_o^2 - d_i^2}{2d_{in}^2} \tag{1}$$

where A_{in} denotes the area of the incoming exhaust gas through both pipes, A_{mix} the cross section in the annular part of the mixing unit, d_{in} the diameter of one exhaust gas supply, d_o the outer and d_i the inner diameter of the annular part of the mixing unit. The CFD-based pressure loss analysis, presented in Sect. 5.1, shows that a reduction of the exhaust gas inflow angle relative to the injector axis α and an increase in the ratio A_r reduces the pressure loss. Based on these findings and incorporating practical limitations by means of production and sizing of the mixing unit, an inflow angle of α = 35° and an area ratio of A_r = 2.4 was used for the experimental configurations in this work, which are described in the following section.

3 Experimental Setups

For the experimental evaluation of the AdBlue mixing unit, tests on laboratory and diesel engine test benches as well as a hydraulic excavator were conducted. The three setups rely on the design parameters developed in Sections 2 and 5.1.

3.1 Optically Accessible Laboratory Urea-SCR Test Bench

For the laboratory investigations, a special test bench with optically accessible dosing and reactor units was used. The rig was recently demonstrated [7] and therefore only a brief description is given for clarity. The bench consists of several sections including gas dosing, heating, AdBlue injection with mixer, and SCR reactor. The mixing unit (Fig. S1, Supporting Information) as well as the reactor are made of quartz glass to check the formation of possible deposits.

The synthetic diesel exhaust gas was adjusted by mass flow controllers (Bronkhorst) and contained various NO_x fractions (340, 500, and 1000 vppm), 20 vol % O_2, 5 vol % H_2O with N_2 as balance. NO_x was dosed as pure NO with 65 mL min^{-1} for 340 vppm, 108 mL min^{-1} for 500 vppm, and 240 mL min^{-1} for 1000 vppm and was mixed with a carrier flow of 2 L min^{-1} pressurized air and then added to the main gas stream. Liquid H_2O was dosed by a pump at a rate of 10 g min^{-1} and evaporated in the gas stream using an external heating device. AdBlue was dosed by a liquid mass flow controller (Bronkhorst) and injected with 30 L min^{-1} pressurized air through a two-component nozzle (Duese-Schlick, Type 970 S8).

The amount of AdBlue was adopted to the NO flow aiming at an equimolar ratio of NH_3/NO_x assuming total conversion of urea to NH_3. For 340 vppm NO_x the AdBlue flow was 24 mL h^{-1}, for 500 vppm NO_x 35 mL h^{-1}, and for 1000 vppm NO_x 70 mL h^{-1}. The temperature in the reactor was adjusted by dosing 206 L min^{-1} pressurized air through two hot air blowers. The total gas flow was 250 L min^{-1} (STP). Before entering the mixing unit, the exhaust flow was split into two pipes with an inner diameter of 10.5 mm. Both pipes were tangentially fixed on the opposite side of the mixer each hitting the flow direction at an angle α of 35°, while the area ratio A_r was 2.4 (Fig. 1, Sect. 2). The resulting hydrodynamic residence time of the gas and AdBlue mixture between the nozzle and the catalyst amounted to approx. 0.08 s (STP).

For the SCR investigations and check of urea deposits on the catalyst, a commercially available $V_2O_5/WO_3/TiO_2$ brick was used. The cordierite-based honeycomb revealed a cell density of 400 cpsi, a diameter of 3 cm, and a length of 15 cm resulting in a gas hourly space velocity (GHSV) of approx. 160 000 h^{-1}. The catalyst was packed into the tubular glass reactor

(d_i = 32.8 mm) and fixed with quartz wool. Temperatures were monitored approx. 2 cm behind the nozzle and approx. 2 cm inside the catalyst (referred to frontside) employing K-type thermocouples. The reactor effluents (H_2O, NO_x, and NH_3) were checked at the reactor outlet with a Fourier transform infrared (FTIR) spectrometer (Multi-Gas 2030, MKS Instruments).

3.2 Diesel Engine Test Bench

The stationary engine test bench implied a one-cylinder diesel engine with direct injection (Yanmar L100N), displacement of 0.43 L, and maximum power of 6.3 kW (3000 rpm). The exhaust aftertreatment system, illustrated in Fig. S2 (top), consists of commercial state-of-the-art devices including a diesel oxidation catalyst (DOC, 300 cpsi, 0.6 L), a cordierite-type diesel particulate wall flow filter (DPF, 300 cpsi, 0.6 L), an in-house made urea dosing system with an air-assisted two-substance nozzle, and an SCR catalyst with Cu zeolite coating (400 cpsi, 0.6 L).

According to the design parameters defined in Sect. 2, the engine exhaust gas was separated by an exhaust splitter (Fig. S2, bottom) upstream to the mixing unit, which implied an inflow angle α of 35° and an A_r ratio of 2.4. The inner diameter of the two inlet pipes was 20 mm each, while the inner diameter of the mixing chamber amounted to 48 mm. The hydrodynamic residence time of the exhaust gas for the transport from the AdBlue nozzle to the hopper of the SCR catalyst was 0.052 s (STP).

The tests were performed under stationary conditions at exhaust temperatures of 165 °C, 175 °C, and 205 °C, which were taken directly in front of the AdBlue nozzle. The exhaust mass flow was always 33 kg h^{-1} (3000 rpm), whereas loads of 20, 25, and 50 % were adjusted resulting in NO_x raw proportions of 200, 220, and 270 vppm. AdBlue was injected to reach a molar NH_3/NO_x ratio of 2 resulting in an AdBlue flow of 48, 53, and 65 mL h^{-1}, respectively. This overdosing of AdBlue was made to critically assess possible deposits originated from urea. Finally, the aftertreatment devices operated at a GHSV of 42 000 h^{-1}.

3.3 Hydraulic Excavator

Real operation conditions were realized by using a Case WX 185 type excavator from CNH Italia (production year: 2008). The hydraulic excavator shown in Fig. S3 included a six-cylinder diesel engine (Case 659TA-M2) with turbocharger, direct injection, displacement of 5.9 L and 118 kW at 2150 rpm. Additionally, Fig. S3 demonstrates the positions of the exhaust aftertreatment devices adopted for the present study.

The excavator offers several predefined load stages (LS), which can be selected by the operator as follows: idle: 840 min^{-1} (LOW-IDLE), LS1: 1150 min^{-1} (LIFT 1), LS2: 1480 min^{-1} (LIFT 2), LS3: 1550 min^{-1} (LIFT 3), LS4: 1650 min^{-1} (ECO), LS5: 1740 min^{-1} (ECO), LS6: 1850 min^{-1} (HEAVY 1), and LS7: 2000 min^{-1} (HEAVY 2). The respective load stage determines the engine speed and the hydraulic pump speed, respectively.

The positions of the commercial aftertreatment devices are demonstrated in Fig. S4 implying a DOC (400 cpsi, 4.0 L), a DPF (300 cpsi, 4.0 L), an in-house made urea dosing system with two-substance nozzle assisted by compressed air, and an SCR catalyst with Cu zeolite coating (400 cpsi, 4.0 L). Temperature and pressure were recorded in front of the DOC (T1, p1), while another temperature was taken in front of the SCR catalyst (T2). The mixing unit was designed according to the design parameters presented in Sect. 2 including an angle α of 35° and an area ratio A_r of 2.4. The inner diameter of the two inlet pipes was 58 mm each, while the inner diameter of the mixing chamber was 136 mm. The hydrodynamic residence time of the exhaust gas for the transport from the AdBlue nozzle to the hopper of SCR catalyst was 0.128 s (STP).

Preliminary tests were performed to collect data on the operability of the application including back pressure and temperature levels of the exhaust gas with the installed mixing tube and the aftertreatment devices, but without injection of AdBlue. For this purpose, the excavator was operating for several hours outdoors under real conditions. This was done by excavating loose soil including grabbing full bucket, swiveling 90°, dumping, and again swiveling 90°. Depending on each load stage (from LOW-IDLE to HEAVY 2) and working method of the operator, the exhaust gas temperature was between 150 °C and 480 °C (T1) and the back pressure within the range of 15 to 100 mbar (p1).

Since the excavator is operating with certain preset load stages, special load stages were checked to achieve an exhaust gas temperature in the mixing tube of around 180 °C (T2), which is required for the validation of the mixing unit. As a result, the load stage HEAVY-1 was selected for the validation tests. This mode provided exhaust gas temperatures in the mixing tube ranging from 180 °C to 200 °C after a certain preheating time. The NO_x raw emissions ranged from 200 to 300 vppm with a mean value of 250 vppm, which was taken to realize a stoichiometric NH_3/NO_x ratio upon the AdBlue injection. The exhaust mass flow was around 400 kg h^{-1}.

4 Numerical Setup

The domain of interest was discretized by an unstructured tetrahedral grid with refinement of near-wall regions by prism layers using approx. 1.5 million cells. The resulting two-phase flow was modeled by a classical Eulerian-Lagrangian approach [22]. The Lagrangian parcels, discretizing the dispersed liquid phase number density function in space and time, were initialized on the nozzle exit using a presumed volume-based Rosin-Rammler droplet size distribution with a Sauter mean diameter of 15 µm. The turbulent flow was modeled by the unsteady Reynolds-averaged Navier Stokes (URANS) equation including source terms for mass, momentum, and energy exchange with the liquid phase incorporated. Turbulence closure was achieved by using the k-ω shear stress transport (SST) model [23].

Note that standard models for single droplet momentum transfer derived from sphere drag and heat transfer from energy balance at the droplet surface with Nusselt correlation from Ranz and Marshall [24, 25] were employed for solving the liquid phase equations. For vaporization, the correlation of Frössling [26] was taken. Since AdBlue contains 67.5 wt % water, the main dynamics of the AdBlue spray was captured by considering pure water. It should be stated that the described modeling strategy is a compromise between accuracy and computational effort to evaluate the flow and spray dynamics, which is the focus of the numerical investigation in this work. More advanced modeling approaches would be needed to describe the detailed mechanism of deposit formation on the surfaces as demonstrated in the literature [27, 28].

The gas phase equations together with the motion of the Lagrangian parcel were solved with the open source CFD package OpenFOAM, version 2012 [29]. For evaluation of the spray evolution, the gas phase (without injection) was simulated until steady state was reached. Based on this flow field, the injection of the liquid phase was simulated.

For the numerical simulations, the operation conditions of the one-cylinder diesel engine rig, characterized by an exhaust gas temperature of 178 °C [21], were taken as reference with an exhaust gas mass flow rate of 42.5 kg h^{-1}. The complete set of boundary conditions is given in the Supplementary Information.

5 Results and Discussion

5.1 CFD-Based Pressure Loss Analysis

Within the analysis presented in this section, the pressure difference between the inlet patch (1.1) and the outlet patch (3) (Fig. 1) was determined by varying the angle (α) of the inlet pipes relative to the injector axis as well as the area ratio (A_r) describing the outer diameter of the mixing unit and the injector mounting to the area of the two inlet pipes. In particular, α was varied from 35° to 60° and A_r from 1.1 to 2.4. Furthermore, five exhaust gas mass flow rates were considered ranging from the reference operation point with 85 kg h^{-1} [21] up to 500 kg h^{-1}, which is specifically relevant for the hydraulic excavator application.

The obtained results are presented in Fig. 2 showing that throughout the cases considered the pressure loss is nonlinearly increased with inclining mass flow rate. Additionally, for the constant area ratio (A_r) of 1.1 the pressure loss is decreased if the angle of the inlet pipes (α) declines from 60° to 45° and 35°, whereas the effect of α grows with the mass flow rate. Moreover, when increasing A_r from 1.1 to 1.7 and 2.4 at the angle of 45°, the pressure difference is clearly reduced. These pressure analyses evidence that the reduction of the inflow angle α as well as the area ratio A_r leads to a decrease in the pressure loss of the mixer. Based on these conclusions and the feasibility of production and sizing, an inflow angle of α = 35° and an area ratio of A_r = 2.4 was considered for the configurations investigated in the following sections.

5.2 Global Flow and Spray Dynamics

The global flow features of the mixing unit are depicted in Fig. 3. The off-centered and angled arrangement of the exhaust gas inflow streams 1 and 2 leads to an angular momentum with respect to the injector axis to the flow, as described in Sect. 2, resulting in a swirl. The swirling flow develops downstream of the injector mounting with a defined main flow direction embossed by the angled exhaust gas inflow pipes. This swirl prevents a recirculation at the end of the injector mounting and an enhanced mixing downstream to the injector. Furthermore, the supply through the two inlet pipes leads to an axisymmetric flow. This is of special importance, since it circumvents a preferred movement of the injector-originated flow towards the walls of the mixing unit.

The spray evolving is illustrated in Fig. 4 presenting three different times after start of injection. The direction of the swirl is indicated by a black arrow. The three time steps, characteristic for the initial temporal development of the spray, show an axisymmetric development over time (from 1 ms to 2 ms after start of injection). Thus, the flow arrangement described in Fig. 3 leads to a symmetric spray evolution without a spray-wall interaction. As a result, the working principle of the AdBlue mixing unit is validated by means of the CFD simulation framework.

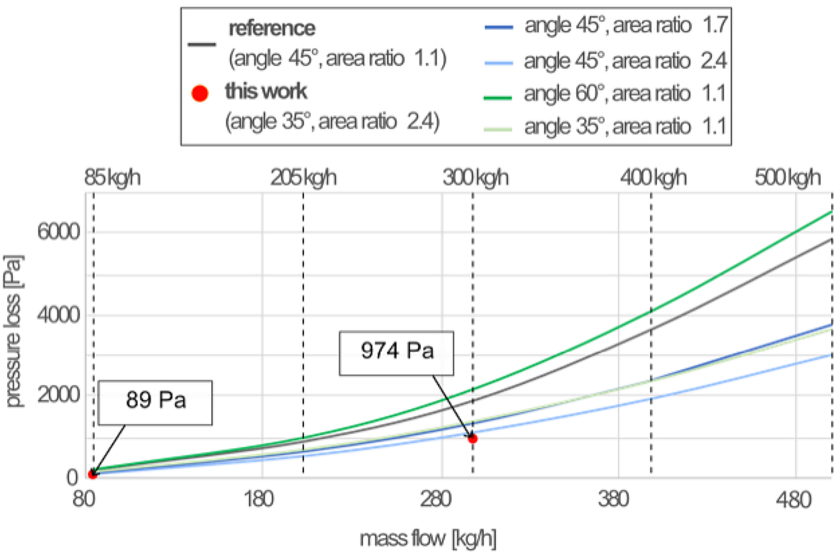

Figure 2. Pressure loss analysis under variation of the mass flow, inflow angle α and area ratio A_r.

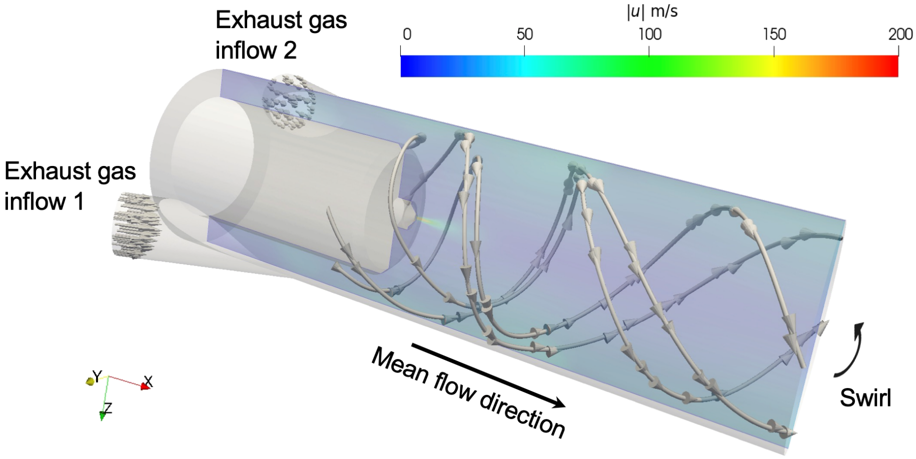

Figure 3. Flow field in the mixing unit.

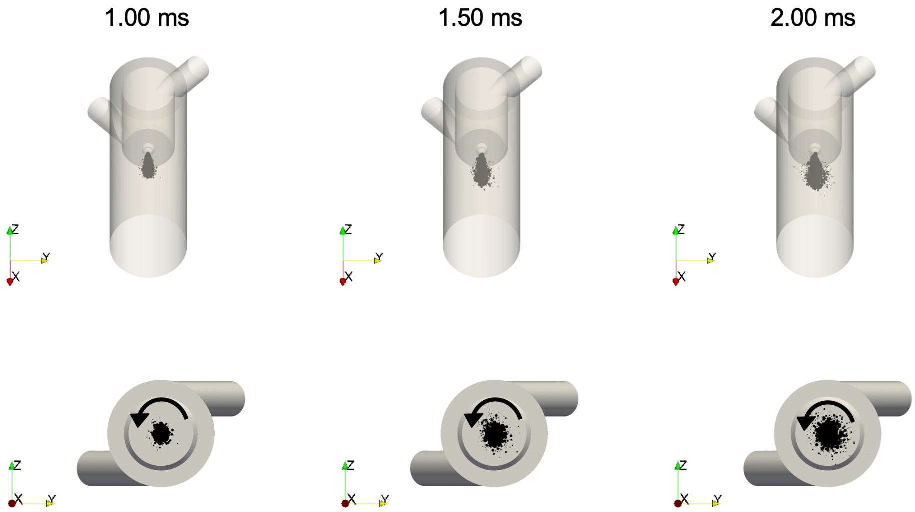

Figure 4. Spray evolution at three different times after start of AdBlue injection. Black dots indicate parcels discretizing the liquid phase, which are scaled by the mass they are representing. The black arrows denote the direction of the swirl.

5.3 Experimental Study Using the Optically Accessible Laboratory Urea-SCR Test Bench

The swirling effect deduced from the CFD simulations and its beneficial impact on the suppression of possible urea deposits was experimentally checked by using the transparent laboratory test bench first. For these tests, the temperatures were varied between 165 °C and 220 °C, as in this range the urea hydrolysis is slow, thus potentially provoking deposit issues. Deposits if formed are promptly observed during the experiments within the optically accessible reactor. The total gas flow was always kept at 250 L min^{-1}, while the NO_x and AdBlue flow was varied maintaining a molar NH_3/NO_x ratio at 1.

Figs. S5 and S6 exemplarily show the NO_x and NH_3 traces for the investigations at 170 °C with 340 ppm NO_x (24 mL h^{-1} AdBlue) and at 220 °C with 1000 ppm NO_x (70 mL h^{-1} AdBlue). In these runs, no deposits were formed in the optical part of the test bench. Here, the obtained NO_x conversions are rather low (36 %) compared to real SCR applications, which is referred to the high GHSV established (160 000 h^{-1}). Note that substantial SCR performance was not in the focus of this work.

For comparison purposes, an experiment with 340 ppm NO_x (24 mL h^{-1} AdBlue), in which a reference mixing unit with an inlet pipe angle α of 45° and an area ratio A_r of 1.1 was used [21], deposits already appeared at 170 °C, while at 180 °C no solids were observed. These results indicate the benefit of the advanced design parameters of the mixing unit (α = 35°, A_r = 2.4) to avoid urea-related deposits. However, at the lowest temperature of 165 °C, some droplets were promptly formed directly behind the AdBlue nozzle, which dried within 15 min time-on-stream and remained in the form of a white solid (Fig. 5). Contrary, no residues were observed downstream to this spot, i.e., neither in the pipes nor on the SCR catalyst.

The FTIR analysis of the found deposit evidenced that it exclusively consisted of urea. This result indicates that the appearance of the residue is ascribed to the evaporation of water, whereas the temperature was not sufficient in this small area to completely convert urea into NH_3 and CO_2. Nevertheless, it is well-known from previous investigations [8] that urea deposits can easily be decomposed without any remaining residues just by raising the temperature in the exhaust gas.

Finally, the studies on the optically accessible laboratory test bench demonstrate that the mixer unit with the design parameters α = 35° and A_r = 2.4 provides reliable AdBlue conversion already at a temperature of 170 °C and above that. By contrast, at lower temperatures "cold" spots can occur, in which the water evaporation is faster than the urea decomposition kinetics thus producing some urea residues.

5.4 Experimental Study Using the Stationary Diesel Engine Test Bench

In addition to the laboratory test bench with the optical reactor (Sect. 5.3), the mixing unit was validated towards the prevention of deposits by using the diesel engine test bench described

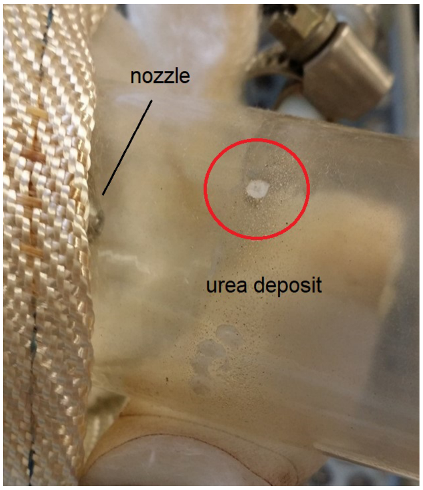

Figure 5. Droplet and solid deposit formation during the AdBlue-SCR test at 165 °C over a time-on-stream of 20 min. Conditions: $y(NO_x)$ = 340 vppm, F(AdBlue) = 24 mL h^{-1} corresponding to 340 vppm NH_3, $y(H_2O)$ = 5 vol %, $y(O_2)$ = 20 vol %, N_2 balance, F = 250 L min^{-1}, GHSV = 160 000 h^{-1}.

in Sect. 3.2. Fig. S7 shows the inlet hopper of the SCR unit (top) and the front side of the SCR catalyst (bottom) after the investigations on the one-cylinder diesel engine test bench at 165 °C (right) and 175 °C und 205 °C (left) each for 30 min. At the temperatures of 175 °C and 205 °C (left), corresponding to engine loads of 25 % and 50 %, no deposits were formed at the AdBlue nozzle and farther downstream. However, when the exhaust temperature was lowered to 165 °C by adjusting an engine load of 20 %, deposits appeared at the exhaust pipe between the nozzle and the SCR catalyst unit, particularly at the inner wall of the inlet hopper and directly in front of the catalyst (Fig. S7, right). FTIR analyses indicated that these deposits were mainly composed of urea with minor proportions of biuret and cyanuric acid.

The investigations performed on the engine test bench illustrate that the optimized mixing unit operates reliably at a minimum temperature of approx. 175 °C, which is close to the test result of the laboratory bench. This comparison points to the feasibility of the scale-up of the mixing unit from an AdBlue flow of 24 mL h^{-1} on the laboratory level to 48–65 mL h^{-1} on the engine test bench.

5.5 Experimental Study Using the Hydraulic Excavator

The principle of the AdBlue mixing unit was finally validated under real-world conditions using the hydraulic excavator in the load stage HEAVY-1 (1850 rpm). Fig. 6 displays the exhaust gas temperature and back pressure for the preheating phase, performed up to a temperature of 180 °C (T2) without AdBlue injection (top), and the subsequent test with AdBlue injection (367 mL h^{-1}) during excavating soil with the hydraulic excavator (load stage: HEAVY-1) (bottom). As described in Sect. 3.3, T1 and T2 represent the temperature in front of the DOC and in the mixing unit, while the pressure (p1) was taken in front of the DOC. The AdBlue injection (400 g h^{-1}) was started once the exhaust gas temperature in the mixing tube (T2) reached approx. 150 °C under operation and lasted a period of approx. 10 h.

Directly after starting the AdBlue injection, the temperature in the mixing tube momentarily dropped to 50 °C, whereas thereafter it remained in the range of 180 °C to 200 °C. As a result of the operation time of 10 h under continuous AdBlue dosing, no deposits were detected in the mixing tube and at the SCR catalyst. Furthermore, the installed exhaust gas system caused a back pressure in the range of max. 100 mbar under all tested operation conditions, which is significantly below the critical value for the engine (250 mbar). Consequently, the performed tests with the hydraulic excavator confirm the reliability of the mixing unit in order to prevent AdBlue deposits at low exhaust temperature (180–200 °C), which are relevant for the efficient NO_x abatement using the SCR procedure.

6 Conclusions

A novel AdBlue mixing unit, recently suggested in a preliminary approach [21], was investigated for the prevention of urea-related deposits in diesel exhaust. The conversion of AdBlue, which is an aqueous solution of urea, into NH_3 and CO_2 is crucial for the reliable application of the SCR procedure, particularly at low exhaust temperatures. The special dosing design is based on a swirling exhaust flow obtained from splitting the total gas stream followed by off-centred introduction of the resulting sub-flows into the mixing unit, in which the urea solution is injected. The produced swirl avoids recirculation of the exhaust flow downstream to the injector and reduces the interaction of AdBlue droplets with the inner wall of the exhaust line, which otherwise can provoke urea deposits.

It should be stated that this strategy to produce a swirl for eliably reliably converting urea is novel and has been practically elaborated in this work for the first time. By contrast, in the literature, mixers with internal swirling devices have primarily been reported so far [15–21].

Furthermore, the CFD-based analysis of the pressure loss showed that a reduction of the exhaust gas inflow angle (α) relative to the injector axis and an increased area ratio (A_r) of the annular part of the mixing unit to that of the inflow stream led to a lower back pressure. The design parameters resulting from these CFD simulations (α = 35° and A_r = 2.4) were further considered for the transfer to the experimental setups and successfully validated using three different levels of complexity, i.e., an optical laboratory test bench, a stationary one-cylinder diesel engine test bench, and finally a hydraulic excavator in real transient operation mode. The upscaling of the mixing unit covered a broad range of the AdBlue flow from 24 mL h^{-1} (laboratory) to 367 mL h^{-1} (hydraulic excavator) indicating the practical relevance of the transfer approach.

As a result of the experimental studies, the tests on the optical laboratory test bench with synthetic exhaust as well as on the stationary diesel engine test bench demonstrated that approx. 170 °C is the lowest operation temperature of the mixing unit without appearance of any urea deposits. Compared to the first approach configuration of the swirling mixer unit [21], the

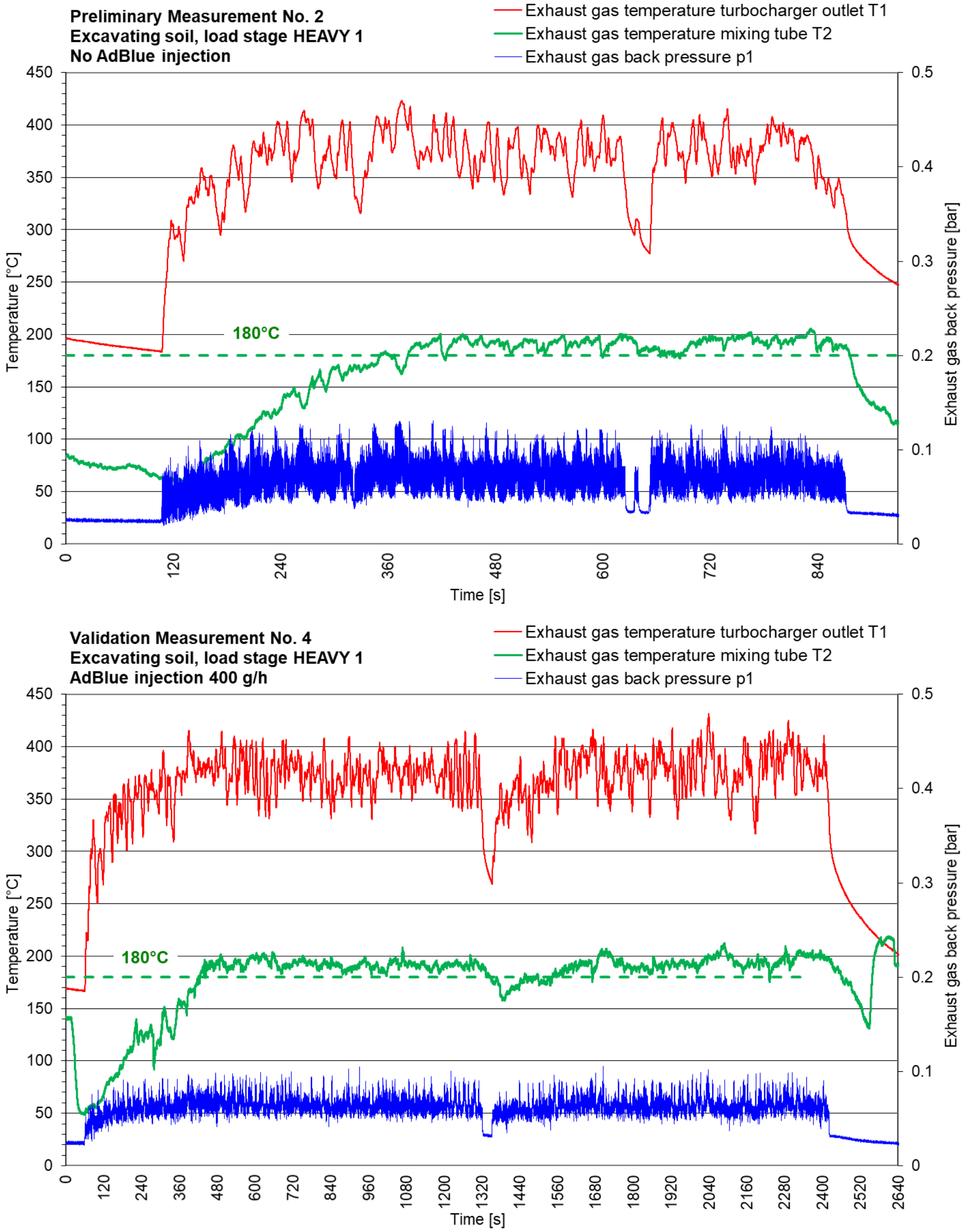

Figure 6. Preheating phase without AdBlue injection (top) and subsequent test with AdBlue injection (367 mL h^{-1}) during excavating soil with the hydraulic excavator (load stage: HEAVY-1, bottom).

modification of the design parameters lowered the reliable operation temperature by at least 20 K. A further decrease in the temperature might be achieved by thermal insulation of the critical areas of the exhaust pipe, where urea is deposited due to cold bridges to the surroundings.

The transfer of the design parameters of the mixing unit to the hydraulic excavator showed that no deposits were observed in the dynamic operation mode of the machine with exhaust gas temperatures in the mixing tube ranging from 180 °C to 200 °C. Thus, the basic principle of the novel AdBlue mixing unit for low exhaust temperatures was proven in practice. Finally, it may be taken into consideration that the lower operation limit of the novel AdBlue mixer, which is 170 °C for the laboratory and stationary diesel engine test benches and 180 °C for the hydraulic excavator, is close to the decomposition temperature of urea, which starts at about 133 °C. Hence, for the evaluation of the operation limits at low temperatures, further operation points should be considered under real working scenarios. In this context, the potential of the mixing stage may also be investigated for other working machines such as delivery trucks, busses, and SUVs.

Moreover, the deposits formed below approx. 170 °C throughout this study mainly consisted of urea, i.e., by-products such as cyanuric acid and biuret were not significantly produced. Therefore, these urea residues can simply be removed to yield NH_3 and CO_2 when the exhaust temperature is inclined. Such scenarios for the removal of pure urea deposits were recently demonstrated [8] and could be considered as an additional back-up strategy when urea is deposited in the exhaust pipe under challenging operation conditions such as high AdBlue mass flows.

Supporting Information

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Symbols used

A_{in}	[m]	area of the incoming exhaust flow of both pipes
A_{mix}	[m]	cross section of annular part of the mixing unit
A_r	[–]	area ratio of the annular part of the mixing unit to that of the inflow stream
d_i	[m]	diameter of injector or inner diameter of tube reactor
d_{in}	[m]	inner diameter of the tangential inlet pipes
d_o	[m]	inner diameter of the mixing unit
F	[L min^{-1}]	gas flow rate
GHSV	[h^{-1}]	gas hourly space velocity
y	[vppm]	volume fraction of gas species

Greek letter

α	[°]	angle of the inlet pipes relative to the injector axis

Abbreviations

CFD	computational fluid dynamics
DOC	diesel oxidation catalyst
DPF	diesel particulate filter
GHG	greenhouse gas
SCR	selective catalytic reduction
VWT	$V_2O_5/WO_3/TiO_2$

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