

CFD simulations and NEDC tests for the original and replacement selective catalytic reduction system

ARTICLE INFO

The purpose of this study was to perform both experimental and computational investigations on the selective catalytic reduction (SCR) system in passenger cars equipped with compression ignition (CI) engines. The study involves a comparison of results obtained for two separate SCR systems: an existing one and a newly developed system. The newly designed SCR system is intended for implementation in the spare parts market (aftermarket) and includes the creation of a custom mixer design. This research analyzed multiple SCR systems and mixers under varying operating conditions. Various factors were considered, including the examination and evaluation of gas distribution and nitrogen oxide reduction. The multiphase computational fluid dynamics analyses were conducted using the ANSYS Fluent software. A detailed assessment was carried out for the sequential processes occurring within the system. The final version of the replacement SCR system was analyzed in relation to the original system supplied by the original equipment manufacturer (OEM). The implementation of the new mixer in the replacement SCR system led to slightly reduced NO_x emissions, as validated by emission tests (NEDC) performed in a car on a chassis dynamometer within a certification unit.

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1. Introduction

1.1. Aftertreatment technologies

Compression ignition engines are extensively utilized in various applications, including off-road machinery, marine vessels, commercial trucks, small commercial vehicles, and private passenger cars. Diesel engines have demonstrated remarkable reliability and performance in the last decade, primarily attributed to their superior fuel economy, increased torque, and reduced CO₂ emissions compared to petrol engines. Despite their advantages, compression ignition engines emit significantly greater levels of NO_x and PM, which pose serious risks to both public health and ecological systems. With the global fleet of vehicles expected to approach 1.3 billion by 2030, the impact of these emissions is anticipated to become even more pronounced.

Emission levels can be mitigated through advancements in primary methods, such as reducing engine-out emissions, the adoption of alternative fuels, or improvements in secondary methods, including the efficiency of emission control systems. To meet the required particulate matter (PM) emission limit, diesel particulate filters (DPFs) are widely applied. On the other hand, nitrogen oxides (NO_x) emissions are effectively minimized in conventional stoichiometric gasoline engines through the use of a three-way catalyst (TWC), which combines oxidation and reduction processes. In contrast, the removal of NO_x emissions using a three-way catalyst in compression ignition engines proves unproductive because of their lean combustion process and the great oxygen concentration in the flowing exhaust gases. As Euro norms become increasingly stringent, the development and adoption of advanced aftertreatment technologies specifically designed for NO_x reduction have accelerated. Among the most effective technologies for reducing diesel engine-out NO_x emissions by over 90% is the

selective catalytic reduction system (SCR), which is the main point of this study.

1.2. SCR system

The SCR system is a solution developed to minimize NO_x emissions to minimal limits. Initially implemented in heating plants toward the end of the seventies, SCR technology was later adopted for gas turbines in the nineties and subsequently for NO_x reduction in coal power plant installations [12]. The initial widespread adoption of SCR technology for cars with compression-ignition engines in Europe occurred in 2005, primarily in trucks [5]. The SCR system utilizes an injector that sprays a urea-water solution, called AdBlue. This solution decomposes into ammonia within the high-temperature exhaust gases, enabling the reduction of nitrogen oxides into environmentally friendly nitrogen (N₂) and water (H₂O) within the catalyst [6]. The typical structure, as well as the phenomena within an SCR system, are illustrated in Fig. 1.

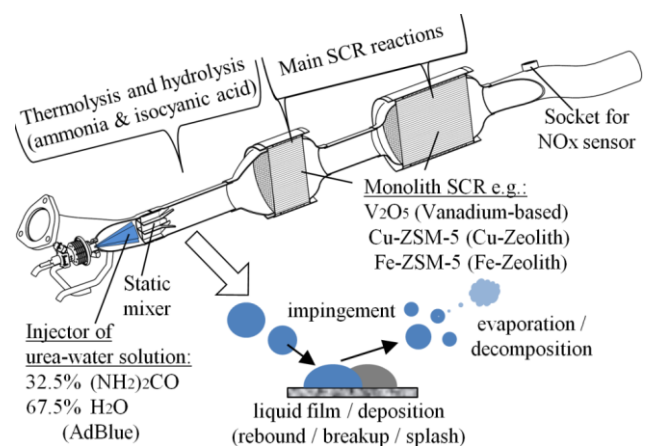


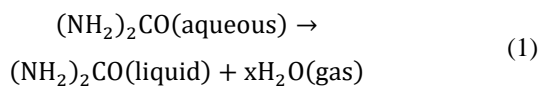
Fig. 1. Construction of the SCR system [10]

Unreacted ammonia can escape into the surrounding air, leading to undesirable secondary harmful pollutants, frequently called ammonia slip. This phenomenon can occur due to excessive injection of AdBlue, insufficient temperatures, a deteriorated catalyst, or inadequate gas mixing within the system. An effective SCR system achieves high NO_x reduction efficiency while keeping ammonia slip at a minimum level, typically in the range of 5–10 ppm [8, 12]. The control mechanism operates in either an open-loop or closed-loop layout. In an open-loop system, a NO_x estimation algorithm calculates the nitrogen oxides levels in flowing gases on the basis of parameters such as engine revolutions, temperature of exhaust gases, and engine load, determining the appropriate quantity of urea-water solution to injection. In the subsequent case, the closed-loop configuration utilizes real-time data from a NO_x sensor, integrated for on-board diagnostics (OBD), to precisely regulate the UWS injection [6, 17].

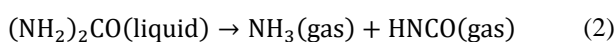
There are three main types of SCR catalysts currently in commercial use, each with distinct properties. Vanadia-based SCR catalysts, among the most cost-effective options, use 1–3% of V₂O₅ as the reactive element, usually supported on titania TiO₂ and combined with WO₃. The addition of WO₃ enhances vanadia stabilization and improves thermal durability. These V₂O₅-WO₃/TiO₂ catalysts exhibit high conversion efficiency in moderate temperature ranges but have limited thermal stability at higher temperatures. Additionally, there is a possibility of vanadium release when operating close to 700°C. Cu-zeolite (Cu-ZSM-5) SCR reactors demonstrate superior NO_x reduction efficiency at lower temperature range, whereas Fe-zeolite SCR reactors (Fe-ZSM-5) are more effective for NO_x conversion at higher temperature range. Additionally, Cu-ZSM-5 catalysts offer the highest capacity for NH₃ storage. However, they are prone to sulfur deposition and necessitate periodic extreme heat for regeneration steps to maintain performance.

Catalyst substrates are typically constructed as monolithic honeycomb structures composed of porous materials (cordierite) with a high surface area. Enhancing cells per square inch (cpsi) from 300 to 400 has a significant impact on NO_x reduction compared to increasing the active side within the SCR reactor [5, 8].

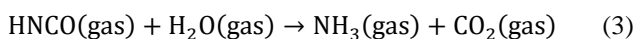
A urea-water solution composed of 32.5% urea and 67.5% demineralized water is sprayed into the flue gas stream. In this technique, water evaporates from the droplets, initiating the following reaction [12]:



Prior to reaching the SCR catalyst, pure urea undergoes thermal decomposition (thermolysis), producing NH₃ and isocyanic acid (HNCO) in the gaseous form [8]:

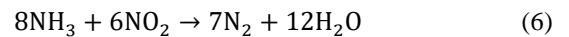
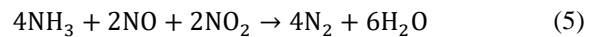
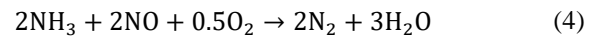


Isocyanic acid reacts with water in a hydrolysis process, leading to the formation of NH₃ and CO₂ [8]:



Subsequently, NH₃ participates in the reaction mechanisms facilitated by SCR reactors. The thermolysis and hydrolysis processes occur at a faster rate than the SCR reactions. The effectiveness of ammonia generation from UWS is highly dependent on the exhaust gas temperature, with the process initiating at temperatures exceeding 130°C [15]. At gas temperatures below 200°C, the decomposition of urea may result in the formation of by-products (cyanuric acid, melamine, ammeline, biuret), which can lead to the accumulation of deposits – a result that is highly undesirable. Consequently, urea injection is initiated only when the exhaust temperature exceeds 180°C [5, 12]. However, full reduction of UWS into ammonia is not accomplished before reaching the catalyst. However, enhancing the hydrolysis mechanism in the gaseous form in front of the reactor entry can be fulfilled through increased temperatures, optimized injection design, efficient mixer configuration, system insulation, or by extending the gas flow path. The quality of AdBlue dosing as well as mixing is a complicated process; however, it may improve reduction efficiency even by 10% [15].

Among these processes, three primary SCR reactions play a crucial role [12, 17]:



The first reaction (4), referred to the 'standard SCR' reaction, is highly effective at reducing NO_x emissions at temperatures exceeding 300°C. In exhaust gases, NO_x primarily consists (over 90%) of NO, which reacts with ammonia in accordance with the 'standard SCR' mechanism [12]. The 'fast SCR' reaction, described by Eq. (5), occurs at a significantly higher rate than the standard SCR reaction. NO_x conversion efficiency can be notably enhanced when the NO:NO₂ ratio is maintained at 1:1 [15]. In diesel exhaust gases, the NO₂/NO_x ratio typically ranges from 5 to 10%. That proportion may be improved by adopting a diesel oxidation catalyst that uses platinum as its active side [8]. The process enables the oxidation of nitrogen oxide to NO₂, thereby improving nitrogen oxides conversion efficiency in the SCR system, especially at lower temperatures. Additionally, the chemical reaction described by Eq. (6) occurs, and it proceeds at a much slower rate than the 'fast SCR' reaction and is even less rapid than the 'standard SCR' reaction. Therefore, it is commonly known as the 'slow SCR' reaction [12, 17].

1.3. Vanadium-based catalyst

The vanadia SCR catalyst contains V₂O₅ (vanadium pentoxide) as its active component and is typically supported on anatase TiO₂ (titanium dioxide), which features a high surface area and a porous structure. It is frequently combined with WO₃ (tungsten trioxide) to stabilize V₂O₅/TiO₂, enhance thermal durability, and prevent catalyst poisoning by SO₂. V₂O₅ offers high catalytic efficiency and cost-effectiveness at a specific concentration [14]. Typical compositions consist of 1–3% V₂O₅ and approximately 10% WO₃ on a TiO₂ support. Kröcher et al. [8] recommend

limiting V_2O_5 content to a maximum of 2% to prevent increased N_2O emissions after aging at $600^\circ C$. In mobile applications, the majority of commercial SCR catalysts typically contain 1.7% to 1.9% V_2O_5 . For improved DeNO_x performance and better capture of urea droplets within the catalyst, increasing cell density from 300 to 400 cpsi is preferred over raising the vanadia concentration to 3% [8]. The active component is either applied as a washcoat on an inert substrate or extruded, ensuring that the substrate walls incorporate the catalyst material throughout their entire structure. For mobile applications, typical cell densities are 300 or 400 cpsi, with wall thicknesses ranging from 4 mil (100 μm) to 8 mil (200 μm) and washcoat thicknesses between 20 and 100 μm [4].

Vanadia-based SCR catalysts generally have an optimal temperature range for maximum NO_x conversion between approximately $250^\circ C$ and $500^\circ C$. At low temperatures (prior to “light-off”), the reaction rate is slow, resulting in low NO_x conversion. At temperatures above $500^\circ C$, NO_x conversion decreases due to the oxidation of NH_3 by O_2 , which interferes with its reaction with NO, leading to an increased formation of N_2O [4, 8]. Raising the V_2O_5 concentration improves the SCR catalyst’s activity at low temperatures. However, this reduces the specific surface area (SSA) of the catalyst washcoat material. For instance, 0.78 wt% of V_2O_5 has an SSA of 87 m^2/g , while 3.56 wt% of V_2O_5 has an SSA of 64 m^2/g . Increasing the wash coat loading from 180 g/dm^3 to 540 g/dm^3 lowers the temperature for 70% NO_x conversion from $275^\circ C$ to $220^\circ C$, but it also increases the wash coat thickness and results in higher backpressure. Additionally, large pores increase the diffusion rate of reactants into the washcoat, but they reduce the catalyst’s specific surface area. For vanadia-based SCR catalysts, an optimal balance is reached when the SSA is around 75 m^2/g , and the pore sizes are about 10 nm. It is also important to note that a high vanadia content encourages the phase transition of TiO_2 from anatase to rutile, resulting in reduced catalyst thermal stability. Therefore, the addition of WO_3 or sometimes MoO_3 (Molybdenum trioxide) to V_2O_5/TiO_2 enhances the catalyst’s activity and improves its thermal durability by stabilizing TiO_2 against phase transitions. With WO_3 , rutile formation occurs at $900^\circ C$ instead of $700^\circ C$. The phase transformation results in a loss of the BET (Brunauer-Emmett-Teller) surface, which is used to characterize the specific surface area. Thermal exposure of vanadia SCR catalysts causes thermal deactivation (loss of TiO_2 surface area due to sintering), leading to a gradual reduction in NO_x conversion and potentially contributing to the volatilization of vanadia from the catalysts [4, 8].

To achieve optimal adhesion of the catalyst layer, colloidal silica is used as a binder, resulting in a quaternary system of $V_2O_5/TiO_2-WO_3-SiO_2$ [8]. Kobayashi et al. [7] discovered that the V_2O_5/TiO_2-SiO_2 catalyst with 10–20 mol% of SiO_2 exhibits higher activity than the pure TiO_2 catalyst. Additionally, the combination of TiO_2 and SiO_2 oxides has a large BET surface area, good thermal stability, and lower activity in the oxidation of SO_2 . Liu et al. [14] also described that adding Si to TiO_2 inhibited phase transformation and increased the number of acid sites (Brønsted

acids) and oxidation properties, thereby improving DeNO_x effectiveness. Various transition metals have been found to be active in NO_x reduction, including TiO_2 -supported V_2O_5 , Fe_2O_3 , CuO , MnO_x , and CeO_x catalysts. Among various metal oxides, pure V_2O_5 or V_2O_5 supported on oxide carriers like Al_2O_3 , SiO_2 , ZrO_2 , TiO_2 , etc., have been extensively explored to improve the thermal stability of catalysts [13, 14].

Vanadia-based SCR catalysts are generally quite resistant to sulfur poisoning [6]. However, under low-temperature conditions, they can become deactivated when operating on high-sulfur fuel due to blockage by sulfate species. The formation of ammonium sulfate is reversible, with decomposition becoming evident above $350^\circ C$. Hydrocarbon poisoning on vanadia-based SCR catalysts is less significant than zeolite-based SCR catalysts and oil poisoning [2, 4].

1.4. Requirements for a replacement SCR system

When the original emission part becomes worn-out or loses its performance, it may be substituted with an after-market replacement pollution control device. To bring a replacement emission part for sale, it must undergo homologation testing in compliance with UNECE Regulation 103 or 715/2007, as revised for vehicle types. These vehicles are checked for pollutants emitted into the environment according to Regulation 83. Such directives specify the requirements that pollution control parts must satisfy and outline the necessary checks for approval. In accordance with Regulation 103, devices of an identical category must not vary with respect to the criteria [3]:

- the number of impregnated monoliths, their construction (cpsi), and material composition
- the kind of active layer, including composition of material and proportion
- the volume of the monolith as well as the proportion of its frontal surface
- diameter, length and construction of the substrate
- the thermal protection (heat shield).

Homologation (approval) of a spare part involves certifying a part (e.g. a three-way catalyst) designed to be installed as a spare device for particular vehicle categories with respect to [3, 16]:

- compliance with pollutant emission limits
- compliance with noise level requirements
- effect on car functionality
- compatibility with the OBD system
- durability (must ensure functionality for at least 160,000 km, in accordance with Euro 5 regulations).

Additionally, UNECE Regulation 103 outlines general requirements [3, 16]:

- the spare part needs to be placed in the same location as the original emission part
- the placement of the exhaust path, O_2 sensor as well as other must remain unchanged
- if the original part includes heatshields, the spare part must have them too
- the spare part must demonstrate durability against corrosion and oxidation.

With regard to emissions, the evaluation involves comparing pollutant emissions of a car equipped with the origi-

nal part and the spare part. Both parts are measured three times in accordance with Regulation 83. A spare part is considered compliant if its outcomes comply with the specified restrictions for each exhaust gas component according to the applicable Euro norm and the rules [3]:

$$M \leq 0.85 \cdot S + 0.4 \cdot G \quad (7)$$

$$M \leq G \quad (8)$$

where: M – the average emission values for a specific toxic compound (NO_x , THC, CO, PM, PN) determined from the results of three measurements conducted with the spare part, S – the average value of a specific toxic compound calculated from the results of three measurements conducted with the original pollution control device, G – the permissible limit of pollutant emissions specified in the vehicle's type approval, adjusted by dividing it by the deterioration factors (Table 1) as defined in UNECE Regulation 103.

Table 1. Degradation coefficients for compression ignition engines effective from the Euro 5 standard

NO_x	HC + NO_x	CO	PM	PN
1.1	1.1	1.5	1.0	1.0

In the context of the on-board diagnostics system, the replacement emission control device must not trigger the Malfunction Indicator Lamp during emissions testing. Additionally, the installation of a spare part within the emission system mustn't negatively impact the car's overall efficiency. As a result, exhaust backpressure measurements are conducted to ensure they do not exceed the maximum value specified by the engine manufacturer. What's more, the power output of a car fitted with a spare part should vary by no more than 5% from the power level of a car equipped with the original emission control device [3].

Regulation 103 requires that pollution control devices undergo preconditioning prior to emissions testing, which involves repeating the Extra-Urban Driving Cycle (EUDC) 12 times within the vehicle. The exhaust system's pollutant emissions are then evaluated in accordance with the test procedures outlined in Regulation 83. The measurements are conducted on cars that have been conditioned for a minimum 6h, ensuring the oil and coolant temperatures of the engine reach room temperature, at ambient conditions of 20–30°C. Emission testing begins with a cold engine startup, followed by warming up the engine and pollution control device by three emission measurements performed within the New European Driving Cycle on a chassis dynamometer. In the case of spare part, the pollutant emissions from the exhaust system, averaged and adjusted by deterioration factors (which reflect the effects of aging rather than durability under real-world driving conditions), must remain within the permissible limits for each pollutant [3, 16].

2. Research methodology

2.1. Research objectives and design

This study aims to enhance the efficiency and cost-effectiveness of SCR systems in cars with compression ignition engines through experimental and numerical re-

search. The research compares the performance of two SCR systems: the existing original equipment (OE VW) system and a newly developed system for the WALKER brand. The developed SCR system is intended for introduction to the aftermarket, which includes the development of a dedicated mixer design. As a result, the research involved analyzing different mixer configurations and evaluating the feasibility of creating a universal mixer suitable for diverse operating conditions of the SCR system.

Numerical modelling using computational fluid dynamics (CFD) tools was applied to minimize experimental research costs, simulate reaction kinetics, and develop comprehensive designs of the complete SCR system. Each component of the selective catalytic reduction system (mixer, injector, reactor) was designed and verified based on experimental data. The confirmed designs were subsequently utilized to design and enhance SCR systems.

The research focused on the selective catalytic reduction system with the OE no. 3AA254400AX, dedicated to the VW Passat 2.0 BlueTDI 103 kW. This model, produced between 2010 and 2014, already complied with the Euro 6b emission standard. Figure 2 illustrates the aftertreatment system presented at the motor show. It is worth noting that the diesel oxidation catalyst (DOC) and DPF filter are integrated into a single unit and were excluded from the validation process, which focused only on the SCR catalyst.



Fig. 2. Emission control system during the automotive exhibition (personal photos provided with permission from Prof. M. Brzeźański)

The selective catalytic reduction system was checked using the suggested mixer prototype, which was designed for simple installation without requiring costly equipment and optimized for universal operation. The prototype mixer was evaluated against the original VW mixer. A summary of all static mixers discussed is presented in Table 2.

The tests were categorized into specific cases, as outlined in Table 3. The performance of the whole SCR prototype was evaluated to that of the original VW SCR system.

The evaluated prototypes featured a vanadium (V_2O_5) catalyst as the active component, deposited and applied on TiO_2 (anatase) and SiO_2 (silica). In contrast, the original VW part utilized a Cu-ZSM-5 (zeolite) catalyst [1]. Com-

prehensive details regarding the SCR catalysts are provided in Table 4.

Table 2. Tested mixers

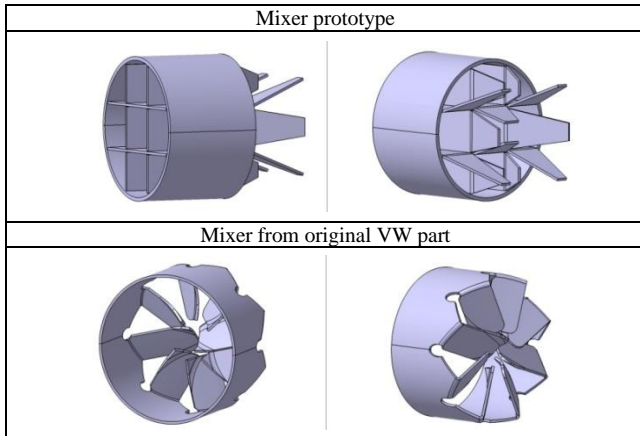


Table 3. Cases studied

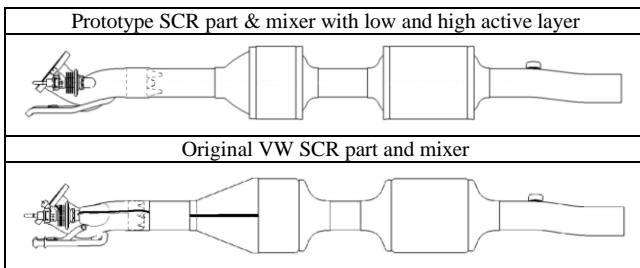


Table 4. Geometrical and chemical properties of SCR catalysts

Part	Box	D × L [inch]	CPSI [1/inch ²]	Type of catalyst	Active layer [%]
Proto with low loading	Front	5.66 × 3	300	V ₂ O ₅ /SiO ₂ -TiO ₂	1.36
	Rear	5.66 × 6	300	V ₂ O ₅ /SiO ₂ -TiO ₂	1.36
Proto with high loading	Front	5.66 × 3	300	V ₂ O ₅ /SiO ₂ -TiO ₂	1.60
	Rear	5.66 × 6	300	V ₂ O ₅ /SiO ₂ -TiO ₂	1.60
Original VW part	Front	5.66 × 3	N.A.	Cu-ZSM-5	N.A.
	Rear	5.66 × 6	N.A.	Cu-ZSM-5	N.A.

Additionally, two fully assembled prototypes were made ready for emission testing in TÜV SÜD Auto Service GmbH, each with different loadings of the active vanadium site. One prototype featured a low loading, while the other had a higher loading. The effect of these active layers was analyzed throughout emission evaluations conducted using the NEDC test on a vehicle test bench with a car for that selective catalytic reduction system.

The prototypes were physically prepared by the Tenneco prototype shop. Based on prototype drawings and the original VW part, the fixture was constructed (Fig. 3). This equipment enables the reproduction of the original VW part's geometry, incorporating various bases crucial for

ensuring proper installation of the components under the vehicle.



Fig. 3. Fixture of the SCR prototype

In Tenneco laboratories, the prepared prototypes were evaluated for pressure drops, gas flow, and NO_x conversion efficiency. The distribution of flow and the conversion of NO_x within the SCR systems were analyzed. The NO_x conversion tests accounted for the AdBlue injected at 5 bar pressure with a frequency of 4 Hz, along with other components of the inlet gases. The applied settings facilitated the assessment of NH₃ uniformity and its distribution, as well as the effectiveness of NO_x reduction within the catalysts. Table 5 provides a summary of the working parameters and the exhaust gas composition used during testing.

Table 5. Inlet operating conditions

Load:	OP 1 High	OP 2 Med	OP 3 Low
\dot{m}_{exh} [kg/h]	541	206	98
T [°C]	501	404	268
NO _x [ppm]	500	128	165
UWS dosing [g/h]	650.5	63.6	38.9
NO/NO _x	0,97		
O ₂ [%]	15.3	16,0	17.0
CO ₂ [%]	2.1	1.8	1.3
H ₂ O [%]	4.8	3.7	2.9
N ₂ [%]	equalized		
NH ₃ /NO _x	0.75		

Comprehensive results from these experimental studies are documented in detail in reference [10].

2.2. Emission tests in the certification laboratory

Emission tests comparing the aftermarket SCR system with the original SCR system were conducted by TÜV SÜD Auto Service GmbH, a certified testing authority in Germany. The tests took place in one of their specialized laboratories. A Volkswagen Passat with engine 2.0 BlueTDI 103 kW (2014 year with emission standard Euro 6b) was selected as the test vehicle and prepared for this study. The vehicle and SCR systems were configured in accordance with an additional gas sampling plan designed for research purposes, as illustrated in Fig. 4.

In compliance with Regulation No. 103 of ECE, obtaining type approval required testing the vehicle equipped with the replacement SCR system in comparison with the original VW SCR system to evaluate both noise levels as well as backpressure. Noise measurements were conducted under both dynamic driving conditions and while the vehicle was stationary. Meanwhile, exhaust backpressure was measured upstream of the SCR system.

These data were collected at the TÜV SÜD Auto Service GmbH laboratory in accordance with Regulation No. 59 of ECE. Following this, emission tests using the new European driving cycle were performed at the second laboratory. This facility has advanced instrumentation, including a MAHA chassis dynamometer, a HORIBA CVS collection system and a pollutant measurement device. The inspections were adapted to the standards outlined in Regulation No. 103 and R83 of ECE as well as Regulation EC No. 715/2007.

Prior to shipment to the research laboratory, the WALKER SCR prototypes were fitted with thermal insulation on the front side, provided by the Culimeta company. This insulation was designed to maintain higher exhaust gas temperatures, which is essential for facilitating the required chemical reactions.

Figure 5 illustrates the proper installation of the tested parts under the vehicle, including gas collecting positions for the ultraviolet tester and quantum cascade lasers as well as for temperature measurement (thermocouples). Additionally, Fig. 6 shows the car ready on a break dynamometer in the lab, set up to measure pollutants using the CVS technique with sampling containers throughout the new European driving cycle.



Fig. 5. Prototype SCR system installed with measuring equipment



Fig. 6. Vehicle ready for the NEDC cycle

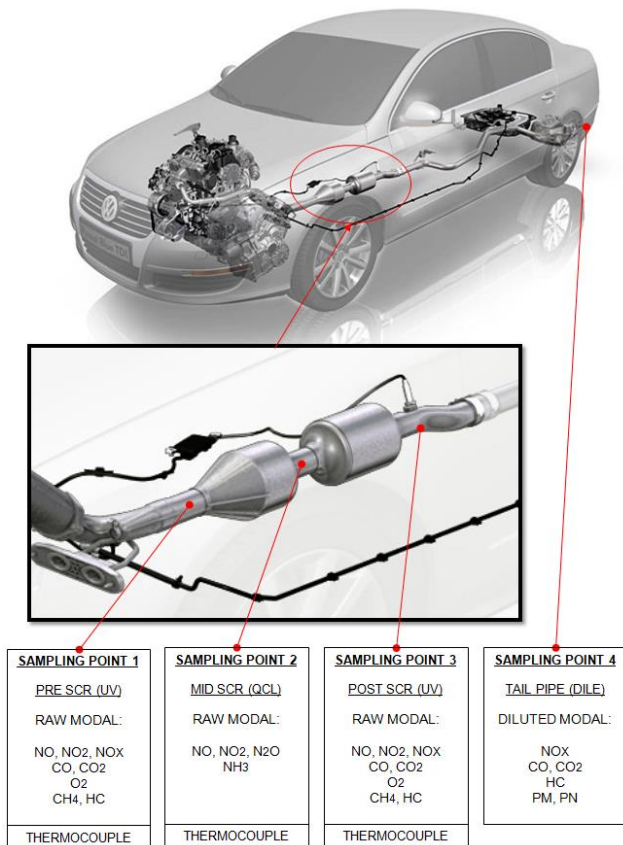


Fig. 4. Measurement points during emission approval tests

3. Results

3.1. Numerical results

The three-dimensional (3D) representations of selective catalytic reduction systems prepared for CFD simulations were created through reverse engineering, following the

methodology outlined in [10]. The computational model was constructed using the commercial software ANSYS Fluent. Individual components of the SCR catalyst, including the injector, mixers as well as reactors, were modeled and verified against experimental data presented in [9, 10]. Upon validation, the improved model was applied to optimize the configuration and performance of the whole SCR part.

The essential calculations required for defining boundary conditions and input data in the simulation software were described in [9–11]. Furthermore, the development of a discrete 3D model for simulation, along with the key configuration and relevant settings in the simulation software, was also detailed in [9, 10].

The numerical CFD simulation results for each case are presented in tabular format, presenting important parameters that define the performance of each scenario to enable comparison. Additionally, graphical representations of the SCR system focus on illustrating nitric oxide reduction (X_{NO} , NO_{ave_out}) as well as the degree of ammonia mixing ($UI_{NH_3_in}$, $CoV_{NH_3_in}$) across different sections of the system.

Figure 7 presents the CFD simulation results for the complete SCR system incorporating the mixer prototype. This article presents the simulation outcomes for operating parameter OP2 (medium load). The simulations conducted for OP1 (high load) and OP3 (low load) indicate that as the flow rate drops (OP1 > OP2 > OP3), the coefficient of variation at the inlet for NH₃ ($CoV_{NH_3_in}$) reduces, suggesting an improved level of NH₃ homogenization. Under high flow conditions (OP1), NH₃ was primarily located in the central region of the SCR system, leading to a significant

NH₃ slip. In contrast, a marginally reduced ammonia slip was noted under low flow conditions (OP3).

Figure 8 presents the CFD simulation results for the original SCR system and static mixer produced by VW. Particular attention is given to the mixer's performance, which demonstrates highly positive outcomes, including a high UI of nitrogen oxide at the outlet (UI_{NO_out}). Moreover, the SCR system does not exhibit significant ammonia slip, as indicated by NH_{3_ave_out} and NH_{3_max_out} values. The main concern is the highest NH₃ content occurring along the outer border of the inlet face of the reactor, which could lead to the accumulation of unwanted deposits in these regions. The mixer design is relatively simple but necessitates the use of high-cost equipment to achieve the desired curved profile. Nevertheless, the original mixer experiences a pressure drop (Δp_{mix}) that is 6 times higher than that of the prototype mixer.

Since the prototype mixer didn't completely reach its intended performance because of unfavorable findings, a decision was made to develop another one, improved mixer construction (Fig. 9). The newly adjusted mixer is composed of a pair of horizontal and a pair of vertical sheets, each featuring curved ends and square cutouts.

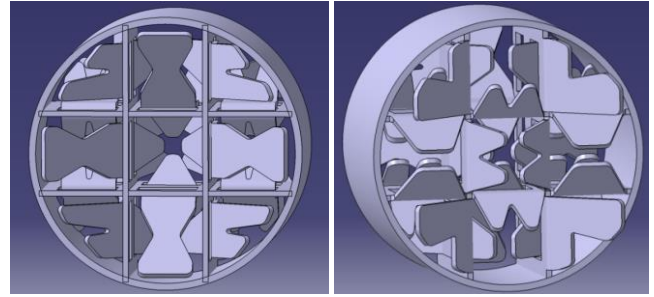


Fig. 9. Optimized construction for improved (newly adjusted) mixer

Three specially designed bent blades are welded on each side of these plates. The overall design of the static mixer is symmetrical, forming an inverted picture in both horizontal and vertical orientations. The mixer construction is considered to be easy to assemble and has universal applicability. Additionally, as urea flows through the mixer, it typically impacts the metal sheets no less than 3 times. This interaction breaks the liquid particles into smaller diameters, enhancing their decomposition into ammonia and improving homogenization within the gas flow.

Numerical simulations were conducted for the newly adjusted mixer for the whole selective catalytic reduction system. In an additional case involving the improved mixer (Fig. 10), a significant enhancement was observed in the UI of nitric oxide at the outlet surface of the tailpipe, exceeding 0.9. In comparison, the case with the prototype mixer achieved a result slightly higher than 0.8. NH₃ distribution at the inlet face of the monolith shows a decrease in the coefficient of variation (CoV_{NH3_in}) and an increase in the uniformity index (UI_{NH3_in}), demonstrating improved NH₃ mixing. Moreover, the maximum ammonia slip (NH_{3_max_out}) remains below 4 ppm, which is an excellent outcome.

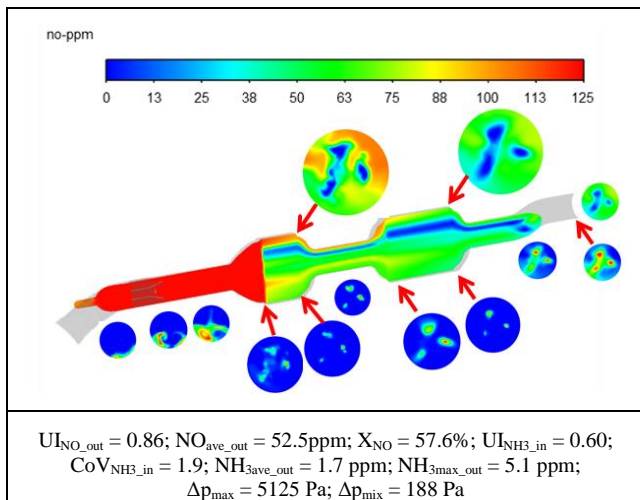


Fig. 7. Nitric oxide conversion and NH₃ uniformity in CFD (case: proto type part & mixer, OP2 – medium)

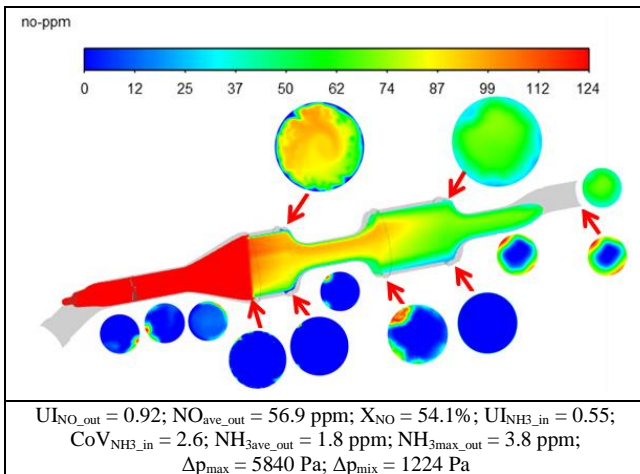


Fig. 8. Nitric oxide conversion and NH₃ uniformity in CFD (case: original VW part & mixer, OP2 – medium)

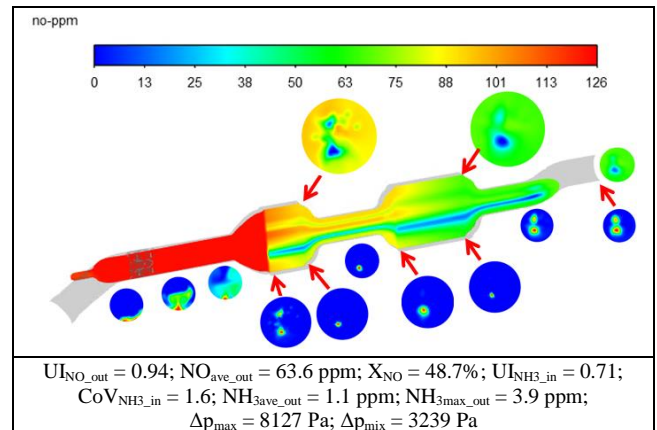


Fig. 10. Nitric oxide conversion and NH₃ uniformity in CFD (case: proto type part & improved mixer, OP2 – medium)

However, this result comes at the cost of a significantly greater pressure drop across the improved mixer (Δp_{mix}), because of the increased construction complexity compared to the prototype mixer. Interestingly, the reduction of NO (X_{NO}) shows a slight decrease, suggesting an improved ammonia distribution to the selective catalytic reduction and a more UI of nitric oxide reduction.

Lastly, an additional SCR system scenario without a mixer was simulated. While the overall nitric oxide con-

version is at a satisfactory value (Fig. 11), the results indicate a lack of uniformity in NO conversion across the SCR catalysts.

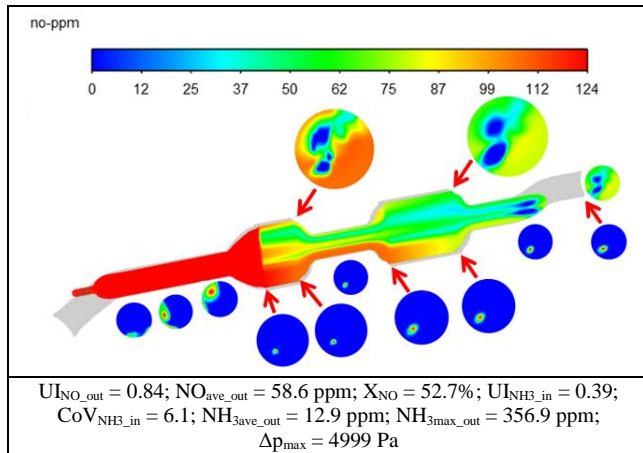


Fig. 11. Nitric oxide conversion and NH_3 uniformity in CFD (case: prototype part without a mixer, OP2 – medium)

NH_3 was mainly accumulated in the upper-left section of the SCR reactor, leading to greater nitric oxide reduction in those fields but reduced NO reduction in the lower right regions. This uneven distribution resulted in a high maximum ammonia slip at the outlet ($\text{NH}_{3\text{max_out}}$), which is further supported by the high coefficient of variation at the inlet ($\text{CoV}_{\text{NH}_3\text{in}} = 6.12$). This approach is rarely applied in practice, as certain regions of the SCR catalyst remain unused, and areas with high ammonia concentrations may lead to deposit formation.

Analyzing the whole SCR part with the newly adjusted mixer more closely, Fig. 12 illustrates the stabilized pressure regions within the SCR catalyst. The highest pressure reaches approximately 8 kPa, compared to about 5 kPa in the system with the mixer prototype.

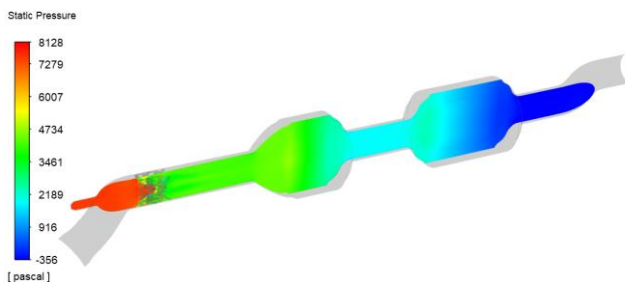


Fig. 12. Static pressure distribution in the case of an adjusted mixer

The temperature regions in the complete SCR reactor for OP2 are presented in Fig. 13. It is observed that the gases are slightly cooled beyond the static mixer and at the inlet surface of the first reactor due to AdBlue dosing. Subsequently, a slight increase in temperature occurs within the SCR catalysts as a result of exothermic reactions.

The velocity vectors in the complete SCR part for OP2 are illustrated in Fig. 14. The highest velocities are observed within the mixer, where turbulent mixing of gases occurs. After the mixer, the average velocities decrease as the flow changes to laminar within the SCR catalysts.

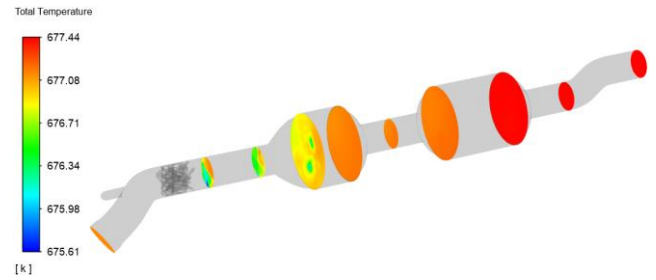


Fig. 13. Temperature distribution in the case of an adjusted mixer

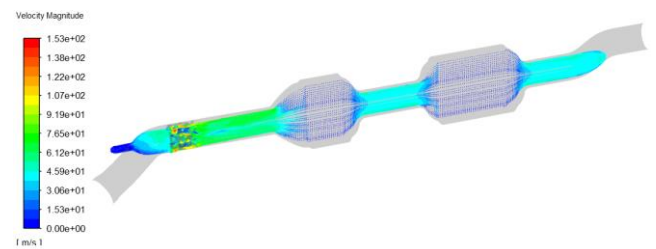


Fig. 14. Velocity vector distribution in the case of an adjusted mixer

The mixing mechanism within the adjusted mixer and the paths of gas velocity as they exit the static mixer are presented in Fig. 15. The improved mixer effectively disrupts the circulation of gases, creating harmonically uniform trajectories throughout the entire pipe. This uniform mixing is highly desirable for optimal ammonia-gas integration.

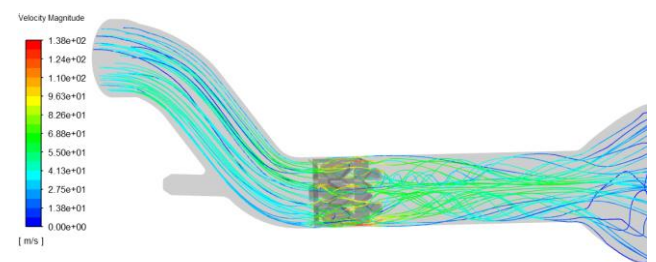


Fig. 15. Velocity and paths of the gas in the case of an adjusted mixer

Figure 16 illustrates the injection of the AdBlue into the inlet of the SCR part and the paths of the liquid particles, highlighting their respective diameters. While the sizes of most fluid particles decrease after passing through the improved mixer, some droplets remain unchanged, likely due to not colliding with the metal sheets of the mixer. Smaller droplets evaporate more quickly, emitting ammonia, while larger droplets tend to collide with the front surface of the reactor and vaporize in that area, resulting in a higher level of NH_3 in that region with insufficient interaction with the gas flow after the mixer. However, the adjusted mixer effectively spreads liquid particles across the entire tube volume.

The evaluation of different mixers in the complete SCR system highlights their impact on NO reduction, mixing uniformity, and maximum ammonia slip. Figure 17 indicates that more advanced mixer designs enhance the UI of NO ($\text{UI}_{\text{NO_out}}$) at the output of the SCR part. It's unexpected that nitric oxide conversion decreases despite this tendency. That occurrence is due to the observation that a less effec-

tive mixer creates greater localized fields of high NH_3 fraction. These concentrated regions lead to the complete reduction of nitric oxide in those areas but also result in excessive ammonia slip. Consequently, the nitric oxide reduction is greater for a mixer with a less complicated design. That is further illustrated by Fig. 18, which shows that a simpler mixer design (allowing “empty passages” of UWS droplets with no collisions with the blades of a mixer) results in greater NH_3 slip, particularly at greater flow rates of gases, such as in OP1. However, this issue was handled with an optimized mixer construction, which achieved a better uniform ammonia distribution, ensuring uniform NO conversion across the entire catalyst volume with marginal NH_3 slip.

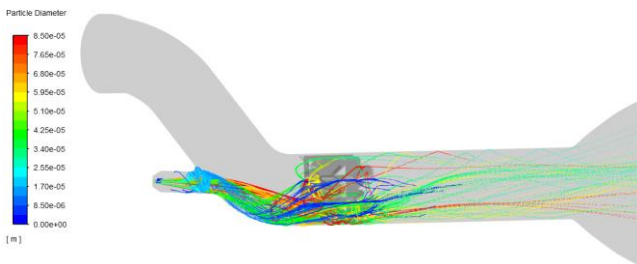


Fig. 16. UWS paths displayed by droplet size for an adjusted mixer

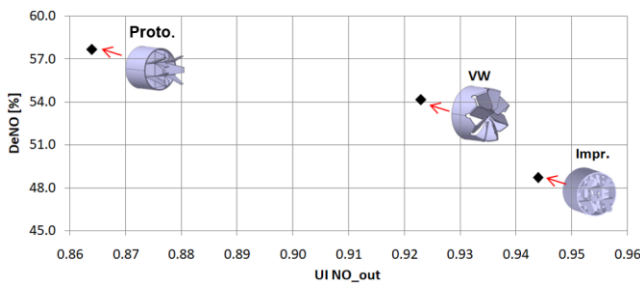


Fig. 17. Comparison of computed nitric oxide conversion and the UI at the outlet (UI_{NO_out}) of SCR system for various mixers

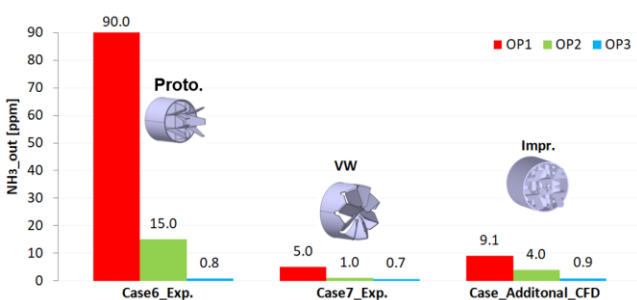


Fig. 18. Maximum ammonia concentration for different mixer designs

Multiple simulations were conducted to evaluate the effect of various SCR system parameters on the results of the simulation. Further CFD analyses were carried out for the entire SCR part with an adjusted mixer under the medium condition (OP2), incorporating modifications to the investigated variable.

The impact of O_2 concentration and subsequently H_2O content in the gases at the inlet on the performance of the selective catalytic reduction system was investigated (Fig. 19a, b). An increase in the oxygen mole fraction from 2%

to 20% (compensated by appropriate nitrogen reduction) enhanced the NO reduction efficiency by approximately 10%. This improvement is attributed to the direct involvement of oxygen in the standard SCR reaction.

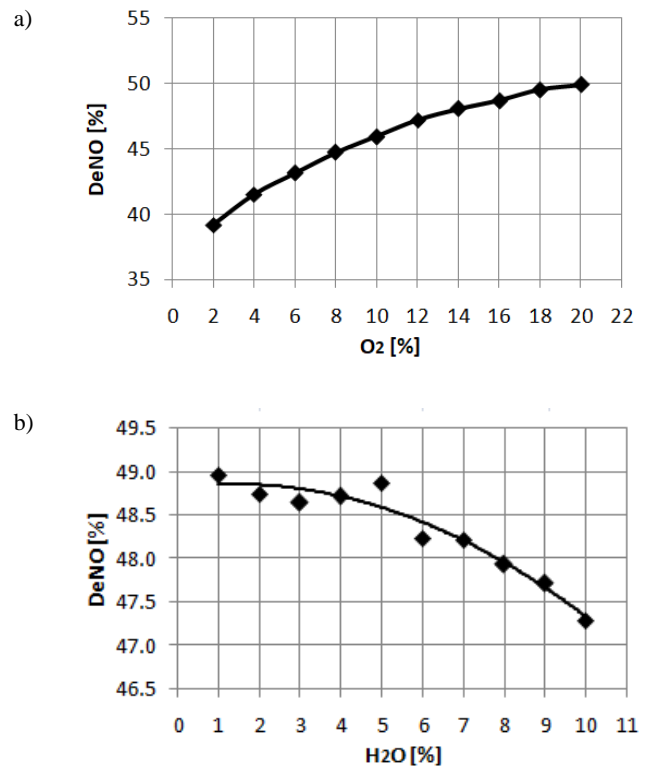


Fig. 19. SCR system with an improved mixer: a) influence of oxygen content on NO reduction, b) effect of water concentration on NO reduction

From another perspective, greater humidity proportions in the exhaust gases lead to a slight decrease in NO conversion, approximately 2%. This reduction is due to water’s participation in the urea-water solution hydrolysis process, where the reaction rate exponent for H_2O is below zero.

The subsequent analysis (Fig. 20) focused on examining the effect of the NH_3 to NO ratio (ANR) on the ultimate NO conversion efficiency in the tested system. It was observed that as the ammonia-to-nitrogen oxide ratio rises, the NO reduction efficiency in the reactor improves. The predictions were validated by the results, showing that ammonia and isocyanic acid concentrations at the SCR system outlet significantly rise when ANR exceeds 1. The best-case scenario appears to be the NH_3 to NO ratio is equal to one, as this minimizes NH_3 slip and prevents the creation of deposits within the system.

The mass flow rate of exhaust gases is another critical factor affecting NO reduction in the selective catalytic reduction system. An increase in the rate of mass flow leads to a decrease in NO reduction efficiency (Fig. 21). This reduction occurs because higher flow rates reduce the duration of gas interaction with the catalysts, limiting the effectiveness of the NO reduction process. Interestingly, high ammonia slip is observed at lower mass flow rates.

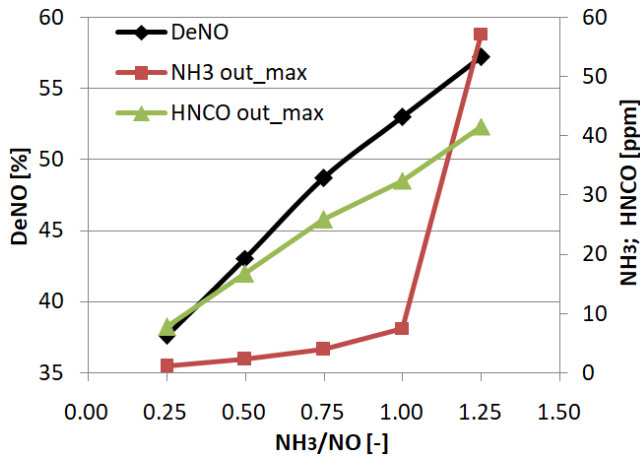


Fig. 20. Effect of the ammonia-to-nitrogen oxide ratio on NO reduction in the SCR system with an improved mixer

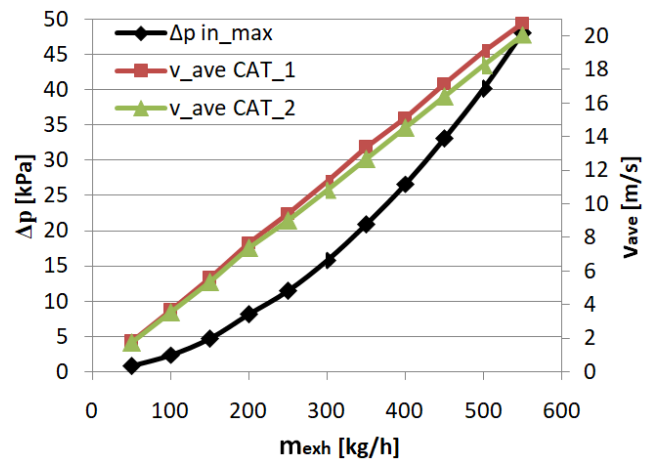


Fig. 22. Effect of the rate of mass flow on pressure drops and gas velocities in the reactors

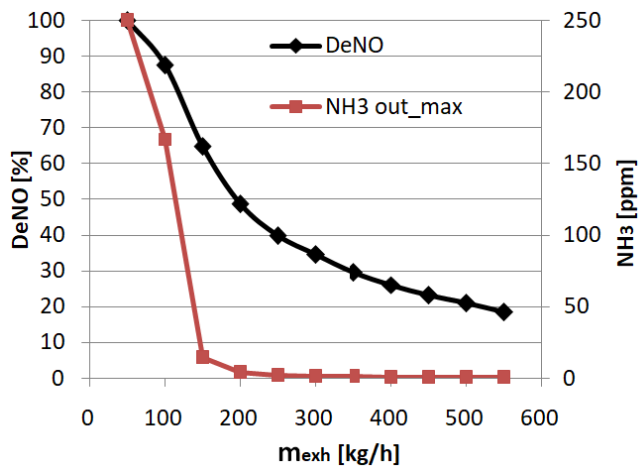


Fig. 21. Effect of exhaust gas mass flow rate on NO reduction in the SCR system with an improved mixer

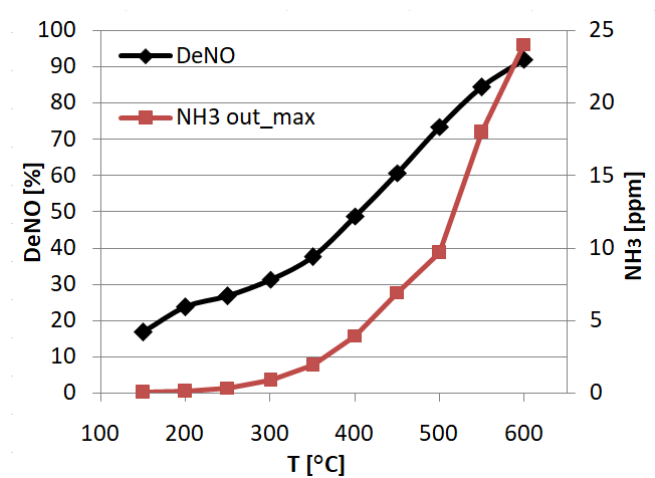


Fig. 23. Effect of temperature on NO reduction and NH₃ slip in the SCR system with an improved mixer

This indicates that at lower flow rates, there is a sufficient period for nitric oxide reduction, but excessive Ad-Blue is dosed. Consequently, the proportion of UWS dosed, which is monitored by the electronic control unit, is adjusted based on the power demand on the engine and the nitrogen oxides content in the exhaust gases.

Growth in the rate of mass flow not only impacts NO reduction but also leads to higher pressure within the SCR system. Furthermore, Fig. 22 illustrates the increase in the average velocity of exhaust gases as they pass through the front and rear SCR reactors as the mass flow rate rises. The average velocity in the rear SCR catalyst (CAT 2) is approx. 1 m/s lower compared to the front SCR catalyst (CAT 1), where the temperature is slightly higher.

The final key factor evaluated in the CFD numerical simulation that impacts the SCR system is temperature (Fig. 23). NO conversion improves as the temperature increases, which is expected due to the favorable conditions for exothermic reactions within the SCR catalyst. Additionally, higher temperatures result in greater ammonia slip at the outlet, caused by more efficient urea decomposition during the thermolysis reaction.

3.2. Emission test results

The process of obtaining ECE Type approval began with assessments of the vehicle's sound level and exhaust backpressure. Following this, emission tests were carried out for both the original VW SCR system and spare part, each tested through three new European driving cycles. Two prototypes of the replacement SCR system were tested, one with low Vanadium loading (RLL) and the other with high Vanadium loading (RHL). The high-loading replacement system was tested in only one NEDC cycle, as the low-loading replacement system successfully passed the tests (all parameters met the criteria specified in Eq. (7) and Eq. (8)). This decision was also driven by the intent to minimize the overall testing costs. To provide a clearer visualization of the required limits and results, the final values for all components of the exhaust gases are presented in Fig. 24a–e.

The analysis revealed that the prototype SCR part with low Vanadium content achieved approximately a 9.5 percentage point improvement in NO_x conversion efficiency over the original system. Furthermore, the high-loading replacement system showed an even greater enhancement, with a 19 percentage point increase. In all tests, the replacement SCR system demonstrated lower emissions of

exhaust gas components compared to the original system. Furthermore, an increased content of the active vanadium layer further enhanced its performance. However, due to the higher cost associated with a higher active layer content, the replacement SCR system finally adopted a lower vanadium loading.

This optimized configuration was sufficient to meet all regulatory requirements during emission tests. Nonetheless, comparing prototypes with different active layer contents provided valuable insights into their influence on final emission results.

The emission results are further analyzed by comparing exhaust gas components and temperatures at measurement locations (Pre-, Mid-, Post-SCR, Tail-pipe) for the original VW SCR part (OE) and the prototype SCR part (AM – the aftermarket replacement with low content of Vanadium) over the 2nd new European driving cycle (Fig. 25). At the start of the NEDC cycle, before the SCR system (Pre SCR), the exhaust gas temperatures began to rise, reaching a maximum of approximately 325°C after the motorway cycle. By the conclusion of the first cycle, the prototype part showed a faster rise in exhaust gas temperature, potentially attributed to better thermal insulation at the inlet. The nitrogen oxide values were generally similar throughout the entire NEDC test for both systems, although higher variations were observed at certain points.

After passing through the 1st reactor, NH₃ slip becomes noticeable for the aftermarket SCR part. While an NH₃ value of 10 ppm is within acceptable limits, higher levels could be mitigated by using a second SCR monolith. At the beginning of the test, the gas temperature at the exhaust in

the aftermarket SCR part was lower. This is likely due to the original VW SCR part, which utilizes Cu-ZSM-5 reactors, gaining temperature more quickly but also cooling down rapidly or possibly having weaker thermal insulation compared to the replacement SCR system. Notably, nitrogen oxide levels downstream of the SCR systems are reduced, particularly during the motorway cycle, where higher exhaust gas temperatures exceeding 150°C improve its performance.

The exhaust gases exiting the tailpipe were diluted at the final stage with air. Throughout the test, a small, predefined amount of the resulting mixture was consistently extracted from the tunnel and collected in measuring bags. All regulatory compliance conditions were fulfilled. The concentration of each exhaust component corresponded to the average concentration measured during the entire testing process. The end result was adjusted according to the concentrations of exhaust gas elements measured, including those obtained with the diluted air. The gravimetric method was used to measure particulate matter, which involved determining the weight of filters where particulates settled.

The achieved compliance with the full scope of applicable standards for the aftermarket SCR part in an authorized certification unit enabled the submission of an approval application. The required documentation for homologation was submitted to the NSAI in Dublin. Upon successful evaluation, the spare part of the SCR system obtained ECE type certification with the number E24103R00/040569*00.

This approval number is engraved on the SCR system, and the replacement part is officially distributed to customers under the WALKER brand.

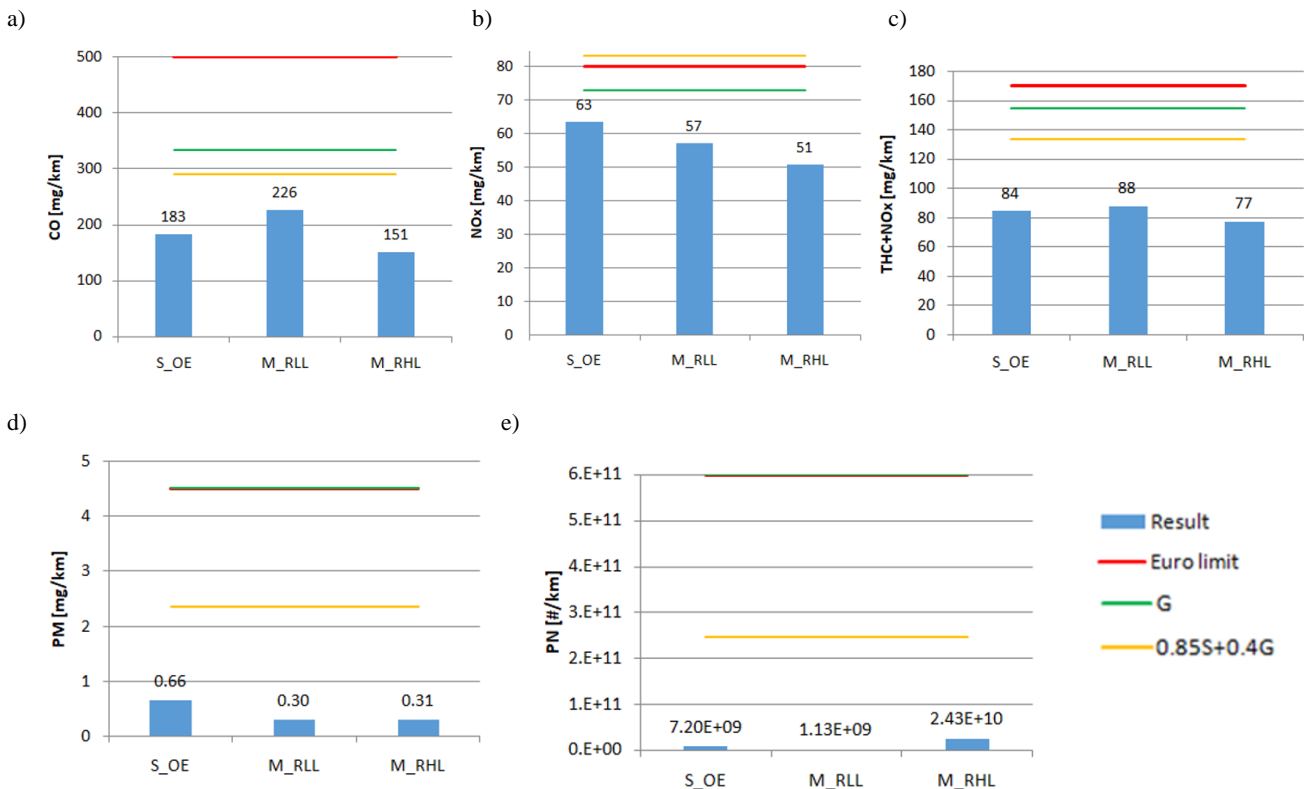


Fig. 24. Emission results for: a) CO, b) NO_x, c) THC + NO_x, d) particulate matter (PM), e) particle number (PN) compared with required limits

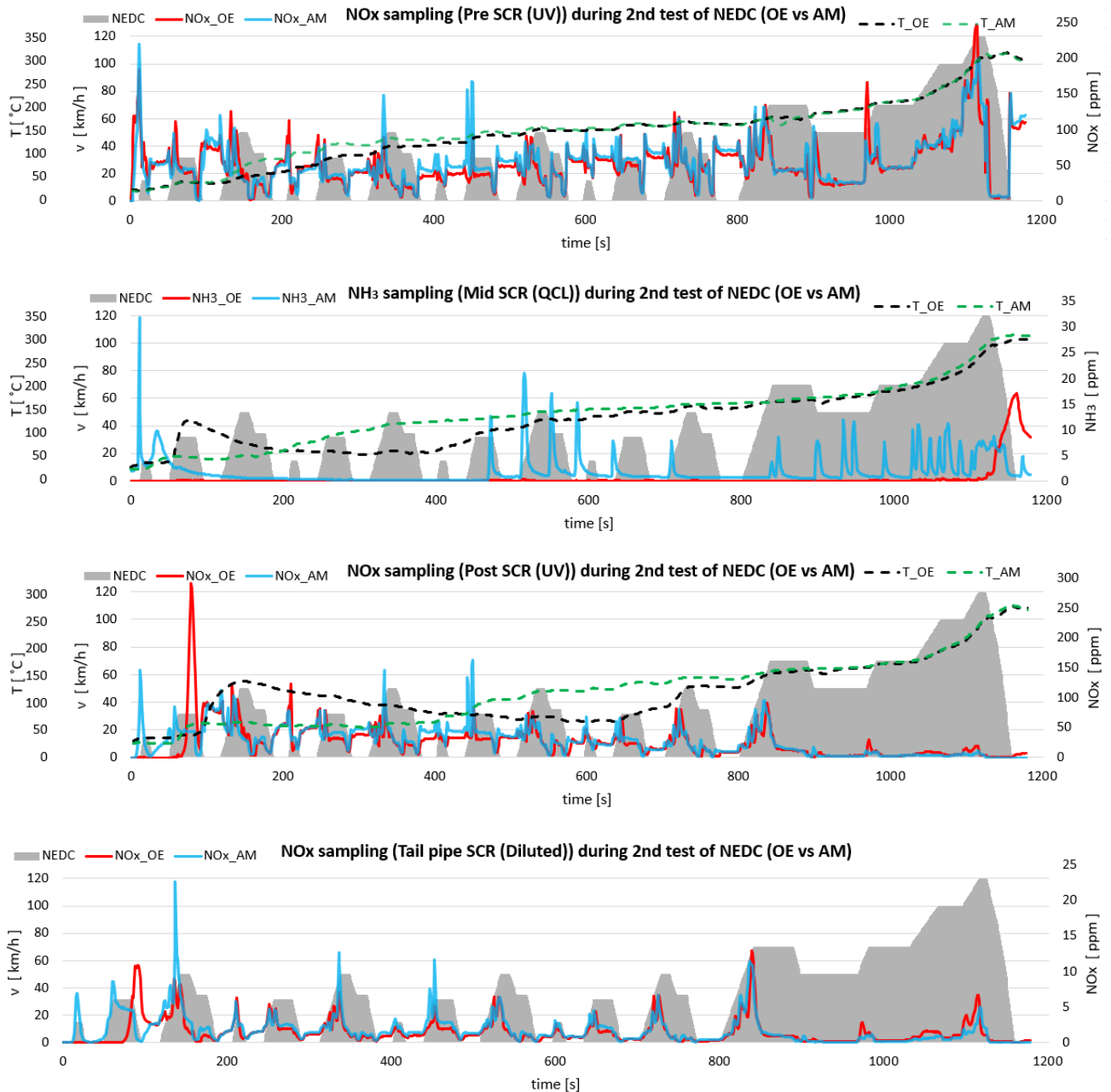


Fig. 25. Exhaust gas components at sampling points (Pre-, Mid-, Post-SCR, and Tail-pipe) for OE & AM SCR systems in the NEDC cycle

4. Summary and conclusion

The research presented within this publication investigates innovative prototype designs for mixers and SCR systems, aiming to enhance their performance. A newly designed SCR system was systematically evaluated against the original system. By analyzing key parameters, the study identifies the mixer configuration that maximizes the operational efficiency of the SCR system. However, simple mixer designs often result in insufficient ammonia release from AdBlue and poor homogenization of gases with NH_3 . This leads to non-uniform nitric oxide conversion within the SCR catalysts and localized high ammonia concentrations, causing ammonia slip. Additionally, such straightforward solutions can promote the creation of unwanted deposit formations within the selective catalytic reduction system.

Static mixers with more advanced designs, such as the original VW mixer, demonstrated a slightly higher pressure drop. Despite this, the design effectively resolved the issue of ammonia slip by achieving enhanced UWS breakdown and more efficient homogenization of NH_3 with exhaust gas flow. Applying the results of the tested mixers and the insights gained during the study, a novel prototype of an adjusted mixer was developed. The adjusted mixer obtained excellent performance in ensuring optimal gas mixing effectiveness. Under all operating conditions, NH_3 slip levels stayed consistently low and within the prescribed allowable limits. However, the main drawback of this design was its relatively high-pressure drop, attributed to its complex structure. Future research will likely focus on redesigning this mixer to achieve a balance between reducing pressure

drop, maintaining effective gas mixing, achieving high nitrogen oxides reduction, and minimizing NH_3 slip.

The developed CFD model accurately predicted the efficiency of the selective catalytic reduction system across different functional parameters. It provides insights into key flow variables, species concentrations, and phenomena occurring within the SCR system. The numerical model was used to examine various cases and setups of SCR systems and proved valuable for future evaluations of other SCR systems and for enhancing the mixer design.

Selecting a different, more cost-effective catalyst type (V_2O_5) for the aftermarket SCR part, instead of the Cu-ZSM-5 as in the original part, didn't reduce nitric oxide reduction efficiency. Dividing the SCR reactor into two units, spaced apart and joined via a short pipe, had a beneficial impact on system performance and improved the nitric oxide reduction rate. This configuration created an extra mixing zone between the catalysts, resulting in a greater homogeneity of NH_3 supplied to the 2nd SCR reactor. Additionally, the smaller size and reduced thermal inertia of the front SCR catalyst allowed it to reach operating temperature (known as 'light-off') more quickly. Tests undertaken in TÜV SÜD Auto Service GmbH proved this finding. The SCR replacement with lower active side content exhibited minimally lower NO_x values compared to the original VW SCR part. Meanwhile, the replacement with higher vanadium loading demonstrated the potential for even greater NO_x

reduction, meeting the stringent standards of the Euro 6b norm.

The aftermarket SCR part, equipped with the mixer prototype, exhibited high ammonia slip from the outlet pipe during tests in a certified emission unit and CFD simulations. While ammonia emissions are not regulated during the new European driving cycle, they may lead to the creation of deposits. These deposits may raise backpressure and contribute to the activity loss of the SCR catalyst. In this work, modifications were implemented to the mixer to reduce NH_3 slip to less than 10 ppm, as proved via numerical simulations. While the improvement was effective, it caused an increased pressure drop because of the mixer's more sophisticated design. An alternative approach to prevent NH_3 slip is installing an ASC catalyst as the last device of the system or implementing a dual-layer ($\text{V}_2\text{O}_5 + \text{Pt}$) on the final segment of the SCR reactor.

The constructed aftermarket SCR part, equipped with the static mixer, achieved full compliance in the authorized research unit, enabling it to receive the necessary approval for potential aftermarket sales.

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Nomenclature

AM	aftermarket	OE	original equipment
ANR	ammonia NO_x ratio	SCR	selective catalytic reduction system
CFD	computational fluid dynamic	$\text{UI}_{\text{NH}_3_{\text{in}}}$	uniformity index of NH_3 (inlet face of monolith)
$\text{CoV}_{\text{NH}_3_{\text{in}}}$	coefficient of variation (inlet face of monolith)	$\text{UI}_{\text{NO}_{\text{out}}}$	uniformity index of NO at outlet
DeNO	average NO conversion	UWS	urea-water solution
EUDC	extra urban driving cycle	v_{ave}	average velocity
\dot{m}_{exh}	mass flow rate of the exhaust gas	X_{NO}	average NO conversion
NEDC	New European Driving Cycle	Δp_{max}	maximum pressure drop
$\text{NH}_{3_{\text{ave_out}}}$	average mole fraction of NH_3 at outlet	Δp_{mix}	pressure drop on the mixer
$\text{NH}_{3_{\text{max_out}}}$	maximum mole fraction of NH_3 at outlet		
$\text{NO}_{\text{ave_out}}$	average mole fraction of NO at outlet		

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