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A methodology to assess mixer performance for selective catalyst reduction application in hot air gas burner

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KEYWORDS

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Abstract The active SCR aftertreatment system is one of the most crucial technology for the NOx reduction of diesel engines. One of the essential parameters of this technology is the urea spray performance on the catalyst. This study presents an experimental and numerical investigation of urea spray behavior used in the heavy-duty diesel engine's selective catalytic reduction (SCR) aftertreatment systems.

The custom test rig is designed and built to simulate exhaust aftertreatment systems of heavy-duty diesel vehicles. Urea injector parameters were observed in this test rig with optic windows for spray and flow visualization. This test rig is available to simulate diesel engines in the sense of exhaust mass flow rate, temperature and spray control unit. The discussion is made about the effects of droplet size of spray and velocity distribution upon flow characterization.

A detailed assessment of the numerical model was presented, and validation was carried out for different interest measurement locations. The predicted droplet size distributions, breakup performance, and velocities are numerically and correlated with the experimental data. The validated model is subsequently used to study the urea-flow mixing dynamics to develop a urea mixer numerically. Test results show that smaller droplets enhance the mixing and thus catalyst efficiency. Mixer design performance can be assessed numerically in the droplet size break up based on the developed criteria called mixer performance criteria. Upstream and downstream of the mixer, droplet size can be extracted from the simulation, and different mixer designs can be compared in terms of the breakup performance.

1. Introduction

In recent years, diesel engines have become the primary power source for heavy-duty vehicle applications. The diesel engine has many advantages over gasoline, such as less fuel consump-

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Nomenclature

1D	One-Dimensional	k	turbulent kinetic energy
3D	Three-Dimensional	*PIV*	particle image velocimetry
EGR	Exhaust Gas Recirculation	*SCR*	selective catalytic reduction
NOx	Nitrogen Oxides	ρ_s	density for isentropic process
PM	Particulate Matter	UWS	urea water solution
CFD	computational fluid dynamics	CO	Carbon Monoxide
SMD	Sauter mean diameter	EC	European Commission

tion, high torque, and thermal efficiency. However, harmful exhaust gases have become the main disadvantage of diesel engines [11]. Emission regulations for diesel engines have become too strict for European standards. European Union registries have led to a significant percentage of reduction of nitrogen oxide (NOx) emissions from Euro 5 to Euro 6 for diesel engines [25,22,14,17].

Diesel engines require an exhaust aftertreatment system since diesel combustion is not sufficient to reduce NOx. Selective Catalytic Reduction (SCR) systems have been designed to efficiently reduce NOx emissions from the combustion system [5]. The SCR is an emission reduction system that includes an injector, catalyst, urea water solution, urea tank, and control system [7,24]. Urea Water Solution, which is called AdBlue in the European market, consists of 32.5 %w urea, 67.5 %w AdBlue [20]. UWS is injected into the urea injector's exhaust system, with a closed-loop controller based on the NOx sensor [12].

In order to produce the reducing-agent, three steps of chemical reactions occur as detailed below:

The first step is to inject the urea-water solution N_2H_4CO through the exhaust system and evaporate the water, then turn the urea into the liquid phase.

$$N_2H_4CO(UWS) \rightarrow N_2H_4CO(lqd) + 6H2O(gas) \quad (1)$$

Liquid urea (N_2H_4CO) decomposes into ammonia (NH_3) and isocyanic acid ($HNCO$) in the exhaust system. The thermolysis reaction is exothermic and occurs in the hot exhaust gas upstream of the SCR catalyst [1].

$$N_2H_4CO(lqd) \rightarrow NH_3(gas) + HNCO \quad (2)$$

The hydrolysis reaction is converted from isocyanic acid to ammonia with water vapor, as shown in Eq. (3). The hydrolysis reaction of urea is exothermic [13,10].

$$HNCO(gas) \rightarrow H_2O(gas) + NH3(gas) + CO2(gas) \quad (3)$$

All chemical reaction conversions are affected by the urea water solution's injection quality and the injection's atomization. There are many studies about SCR in spray effect in the literature [9]. However, studies in the literature have not studied the effect of deposit accumulation and urea droplet diameter on catalysts' efficiency [16].

The exhaust flow affects the spray structure, and mixing is very important for the SXR performance. While it is necessary to focus on the effect of injection parameters on SCR, most SCR studies focus on the exhaust and urea distribution within the exhaust system. Mixing performance involving urea spray has been achieved with simple test benches and limited experimental test results [32]. Besides, fundamental aspects of droplet impingement and mixing processes are not adequately discussed in the literature. The small number of studies on these topics do not cover all diesel exhaust conditions [21]. The variety of SCR injectors in use today with many different parameters makes the problem even more complicated [15].

Many studies have focused on evaporation and mixing in the experimental test setup before doing CAE studies. The study presented in the literature experimentally investigated spray behavior in optical access test equipment when examining droplet evaporation [23,19,18]. These types of studies bring complementary information about flow and spray structure, along with detailed test results.

UWS evaporation and decomposition are among the important steps in the SCR system process, and experimental and numerical studies related to these should be conducted. Depending on the temperature of the urea water solution and the spray diameter, ammonia decomposes [6]. Large droplets will increase the evaporation time, while low exhaust temperature will reduce the evaporation rate. These two parameters harm the evaporation rate. Injection parameters such as the droplet size effects of UWS on system performance were investigated by simulation and experimental methods [8].

Literature studies are carried out under two main headings: the CFD model's simulation methodology and the exhaust system's experimental verification. Mixer development studies are based on trial and error due to the inadequacy of experimental and simulation methods. Experimental and numerical parameters for the mixer selections are not developed.

This study was carried out to analyze the performance of urea droplet breakdown, which is the mixer's main task compared to different mixer performances. Experimental and numerical studies have been conducted to validate droplet breakup performance for SCR mixers. The PIV method measured the urea injector's spraying behavior on the hot gas test bench on the mixer. In addition, the optical window located after the SCR mixer was used to examine the mixer's urea and exhaust gas dispersion performance at different temperatures and mass flow rates on the burner.

A detailed numerical model of the selective catalyst reduction system was created by conjugate heat transfer, sputtering, and chemical reaction modeling. Experimental results have verified this detailed model. The validated model was then used to realize different mixer efficiency in terms of droplet size.

The main contribution to the literature is to provide metric development of exhaust aftertreatment for CFD to develop a mixer and compare. This developed metric is called the breakup index of mixers.

2. Experimental investigation

In dynamometer tests, it is challenging to visualize the spray pattern in the exhaust aftertreatment system due to the particle matters from combustion and fluctuations in exhaust pressure from the in-cylinder movement. Therefore, a hot gas test bench in Fig. 1 was designed and constructed to visualize the urea spray, flow pattern, and deposition accumulation for this study. This system is a custom-designed system that provides controlled exhaust flow, temperature, and NOx concentration for heavy-duty vehicle exhaust development and research. It consists of a natural fired burner with a high flow dilution system and heat exchanger system for temperature control, NOx dosing system, urea dosing system, and the test catalyst section. The urea dosing system is controlled by the DSpace control system, integrated into the burner automation system [4]. The calibration strategies of the urea injector are developed on the Simulink. The simulink model can control the injector, flow test bench, and NOx dosing unit [26].

In this study, mixer performance was investigated in the hot gas test bench. Promising optical techniques were used to obtain flow velocity vector, spray characterization, and deposit formation through the mixing tubes' glass window.

The test section is the component from which the spray was analyzed. Therefore, its layout can be easily reconfigured to simulate the different designs of the exhaust pipe. The configuration used in the experiments consisted of an S-shaped tube and an approximately cylindrical tube (see Fig. 2).

The urea-water injector is located at the end of a long tube from the hot gas generator. In addition, there is a tube to which the mixer can be attached downstream of the injector, followed by the optical section. In this way, injector performance and mixer performance can be monitored from the optical section.

The optical mixer tube provided visual access to the section of the glass pipe. The mixer tube's three flat windows were made of 3 mm thick quartz glass installed downstream of the mixer tube before a 90° bend. Thus, it is possible to introduce the light axially down along the length of the mixer tube or to obtain the upstream images inside the mixer tube utilizing this window. In order to prevent leaks, all joint surfaces are sealed with high-temperature seals.

In this configuration, the optical mixer tube can operate safely at exhaust gas temperatures above 500 °C. Fig. 3 shows an optical tube with three windows.

532 nm power laser pulses are used during PIV studies. Two opposite glasses were opened to the pipe for the laser beams to leave the test piece without breaking inside the pipe. A single glass was opened at 90 degrees to the other two glasses in the pipe to follow the camera's laser beam. It comes to the laser pipe horizontally, as seen in Fig. 3.

On the other hand, the optical test bench in Fig. 4 is designed to measure the injector's spray data experimentally by optical measurement techniques. The size distribution, diameter (SMD), and Dv90 of the spray droplets, including Sauter, and the droplets' initial velocity can be determined from this measurement.

3. Numerical setup

Simulations were performed with the commercial CFD code Star-CCM. The pipes' outer walls are modeled with a low heat transfer coefficient and constant ambient temperature represented in the stationary environment. SCR catalysts are modeled as catalytic porous mediums. The coefficients were obtained from the pressure measurements made on the test rig.

While developing a CFD model in SCR exhaust applications, it is necessary to complete the appropriate turbulence model study to solve the correct flow distribution. First, the k-e-RNG model, the most straightforward turbulence modeling approach, wastried to experiment with the Reynolds stress model.

For inline exhaust aftertreatment systems, simulations of urea-water-solution injection and ammonia conversion are presented. The developed 3D numerical model accounts for all relevant physical effects. The multi-modeling steps were

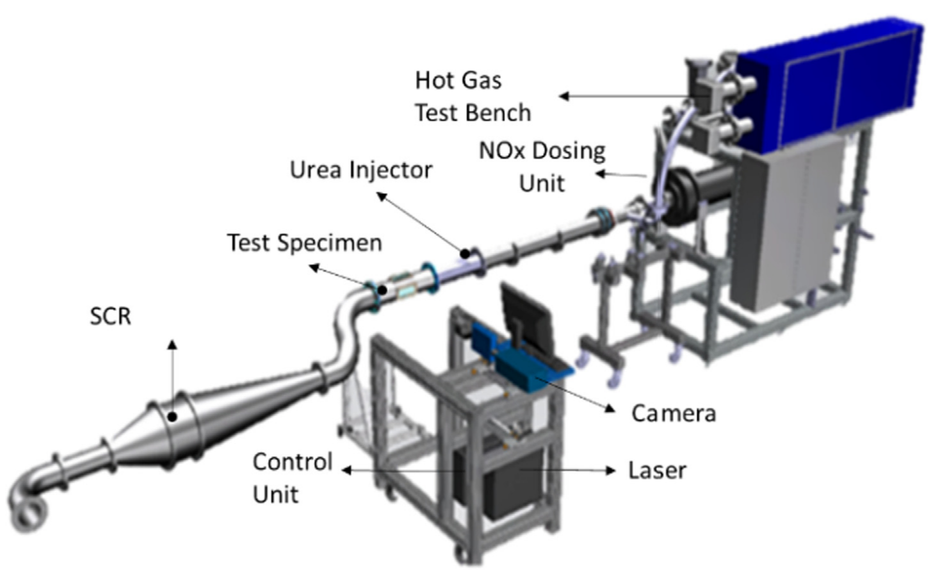

Fig. 1 Exhaust Aftertreatment Test Rig.

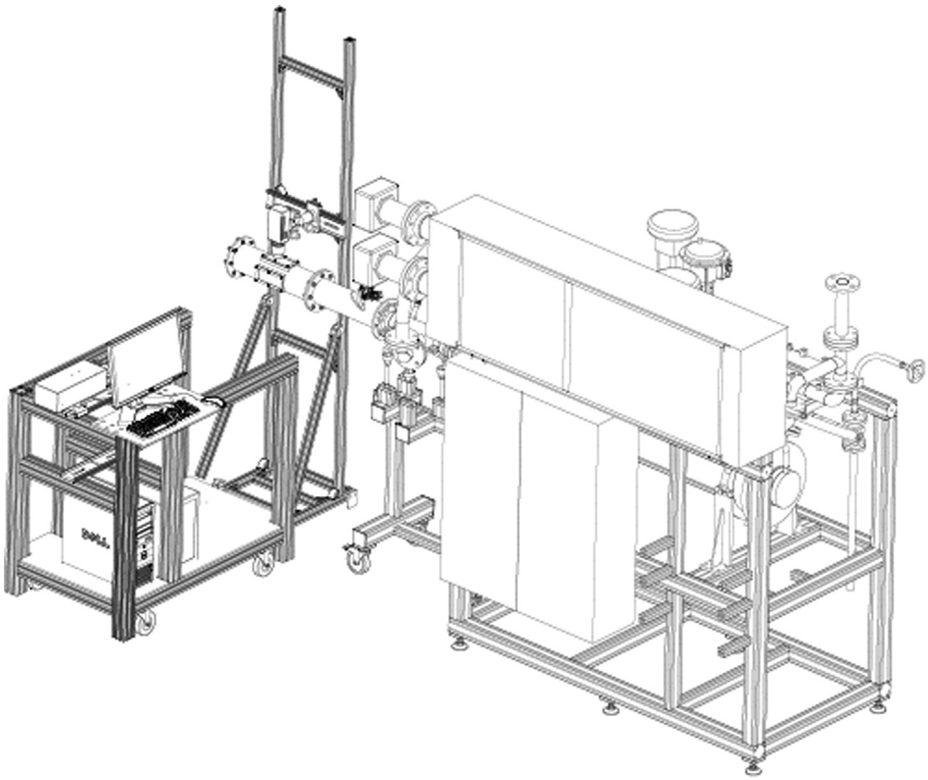

Fig. 2 Optical Test Bench for Exhaust Aftertreatment.

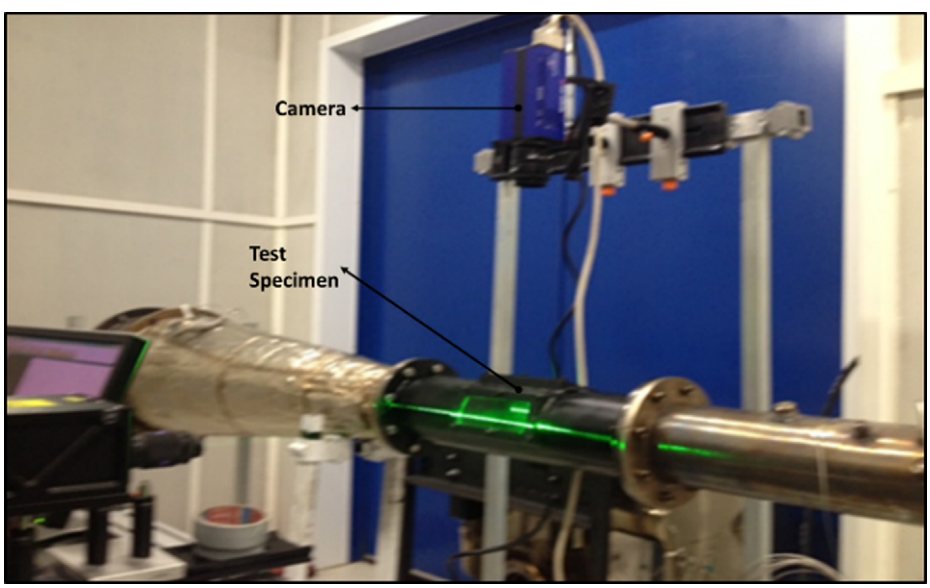

Fig. 3 Optical Test Bench for Exhaust Aftertreatment.

correlated based on each physics literature data, such as the decomposition process. The spray and reducing agent distribution were correlated within the literature work. The influence of flow conditions, exhaust system properties, and spray parameters on the film formation were to be evaluated with the developed simple models. The derived models, including flow field, spray propagation, and chemical reaction from validation works implemented in the Star-CCM. This detailed CFD model predicts deposit location and deposit volume concerning the reducing agent's spatial distribution upstream of the catalyst.

The study focuses on mixing exhaust gas and urea spray distribution upstream of the SCR substrate. Therefore, the geometry used for the simulations is only downstream of the diesel particulate filter exhaust gas system. The flow distribution was almost uniform as %99 after the DPF due to the wall

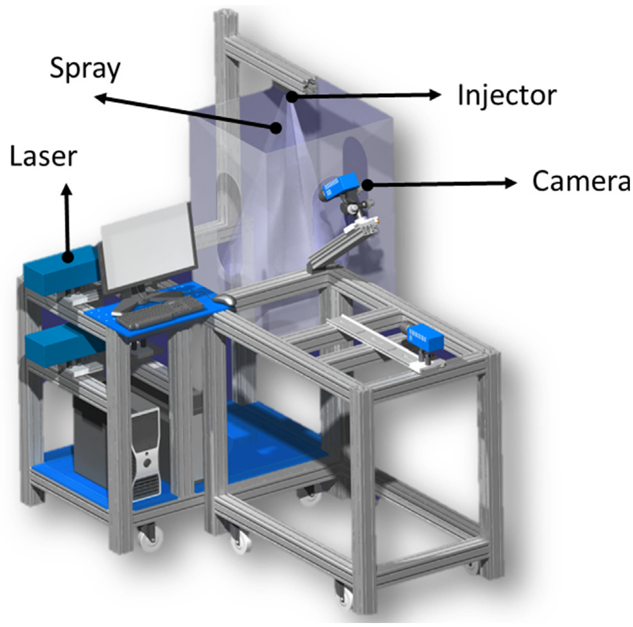

Fig. 4 Spray Test Bench for Exhaust Aftertreatment.

filter effect. Therefore, we can assume homogenous flow distribution at the inlet.

The geometry of the inline exhaust aftertreatment system is displayed in Fig. 5. The CFD model consists of straight pipes, injectors, and mixers, located just after injection. The quartz pipe or three-window pipe is assembled after the mixer. The S-bend pipe and inlet cone are assembled before the catalyst. The solids region of the mixer and the s-bend tube were modeled for conjugate heat transfer modeling, the agitator and s-bend are critical regions for accumulating the deposit, and the tubes have a 130 mm diameter circular cross-section.

The injector, which has three holes, is used for this test. All the parameters are extracted from PIV results, such as spray, cone angles. The initial velocity of the spray and droplet distribution is also delivered from PIV. These results are derived from a spray test bench.

The mesh is created CCM with 3 million elements, including two prism layers around the mixer region to resolve the near-wall conditions. The mixer wall and pipe wall are modeled as solid for conjugate heat transfer. Fig. 7 shows the computational domain of the inline exhaust aftertreatment system. Following the mesh insensitivity study, a base size of 2.5 mm was chosen. In addition, local improvements were made in the mixer area to achieve better results for a more exact simulation of the transition between the viscous substrate and the turbulent layer. The hexahedral is used for the catalyst region. Porous media with one direction flow is used.

The most crucial parameter is spray distribution in SCR simulations. Flow field and temperature should be resolved correctly to determine spray distribution. Therefore mesh types and resolution are prior for SCR simulation. Temperature and pressure drop values of the experimental setup were extracted as reference values. All cases are summarized in Table 1.

Mesh independence cases are carried out in three regions; pipes, mixers and injector region. Global mesh numbers with different mesh types are set from 2 to 3,5 million for all the cases. Since flow and spray behavior is critical, injection and mixer regions are refined. Case 9 was selected for modeling works. Case 9 has the optimum settings for pressure and temperature correlation.

4. Results

A urea injector sprays UWS (32.5% solution) into the pipes. Window glass pipes are used to provide optical access. A diagram of the injection section and the optical arrangement is presented in Fig. 6. Dashed rectangles define optical diagnostics used in both PIV visualization and shadow plotting techniques.

Recirculation zones are created due to the complex mixer structure above the pipe window. The highest fluid velocity occurs at the center of the tube just behind the mixer. Mix blades create vortex and recirculation that can be captured with numerical and PIV measurements (see Figs. 8 and 9).

The flow visualization is completed before the PIV testing that is shown in Fig. 10. The signals are output to a PIV laser and a CCD camera by the developed injection control system for synchronization. In addition, many instantaneous sampling data were collected and post-processed to generate a velocity vector. In this way, the recirculation space can be obtained above and below the pipe window.

Fig. 11 shows the velocity vector in the pipe window. High speed was achieved in the center of the zone. A velocity of 13 m / s is achieved.

Velocity fields are examined in detail. The RSM turbulence model predicts that the flow circulation upstream of the catalyst is in good agreement. However, the k-e turbulence model cannot predict the vortex region upstream of the mixer in Figs. 12 and 13 (See Fig. 14).

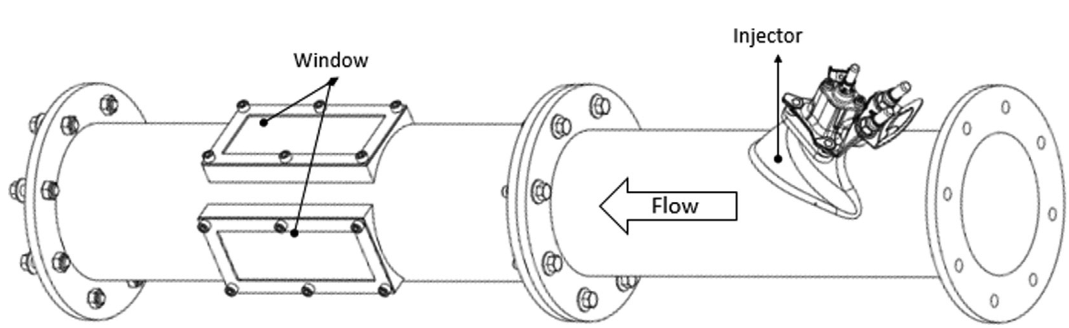

Fig. 5 The geometry of the inline exhaust after-treatment.

Table 1 Mesh type and number sensitivity.

ID	Mesh Type	Number Cells (million)	Level Injection	Level Mixer	The temperature at the Inlet of the Catalyst (0C)	Pressure Drop of the System (mbar)
1	Tetra	2	1	1	698	136
2	Tetra	3,5	1	1	685	133
3	Tetra	5	1	1	680	128
3	Tetra	5	2	2	675	123
4	Poly	1,5	1	1	620	93
5	Poly	2	1	1	622	101
6	Poly	2,5	1	1	626	104
7	Poly	3	1	1	627	108
8	Poly	2,5	2	1	627	108
9	Poly	2,5	2	2	627	108
Ref	Experiment				630	112

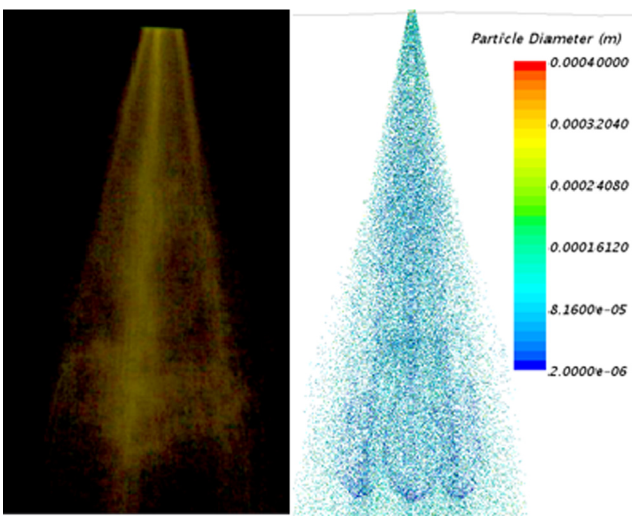

Fig. 6 The spray distribution of the test bench and CFD.

The velocity vector at the inlet cone was observed in Fig. 13. Due to the large diameter of the inlet cone, a low-velocity vector was observed. However, k-e predicted vortex structure for the flow field on the upper surface of the pipe.

Velocity vectors and eddies were observed in the input cones for both turbulence models. However, the RSM model predicts a wider vortex. This recirculating flow area of the pipes affects SCR performance due to poor velocity distribution. It is difficult to measure the flow field distribution with the hot wire sensor in that area. Numerical simulation with PIV correlation and temperature distribution correlation predicts all flow field properties. The velocity, temperature, and ammonia distributions were removed 5 mm above the catalyst.

Fig. 15 shows spray injection of UWS into the gas stream. The gas momentum deflects the spray droplets downstream towards the SCR catalyst, wherein separate drop plots follow the gas flow streams. CFD spray models were developed to predict the spray transport event within the pipe. Spray modeling has been correlated with PIV test data and literature study. This correlation has been applied in the current model. Droplets are modeled as clusters of droplets that interact with the exhaust gas through mass distribution, evaporation, and heat transfer. This number of sets has been studied for precision on the result. 80 k clusters are used in the current model.

CFD shows that the axial acceleration of particles at higher exhaust flow rates tends to spread the spray's effect over a large area downstream of the pipe, thus reducing urea's flux

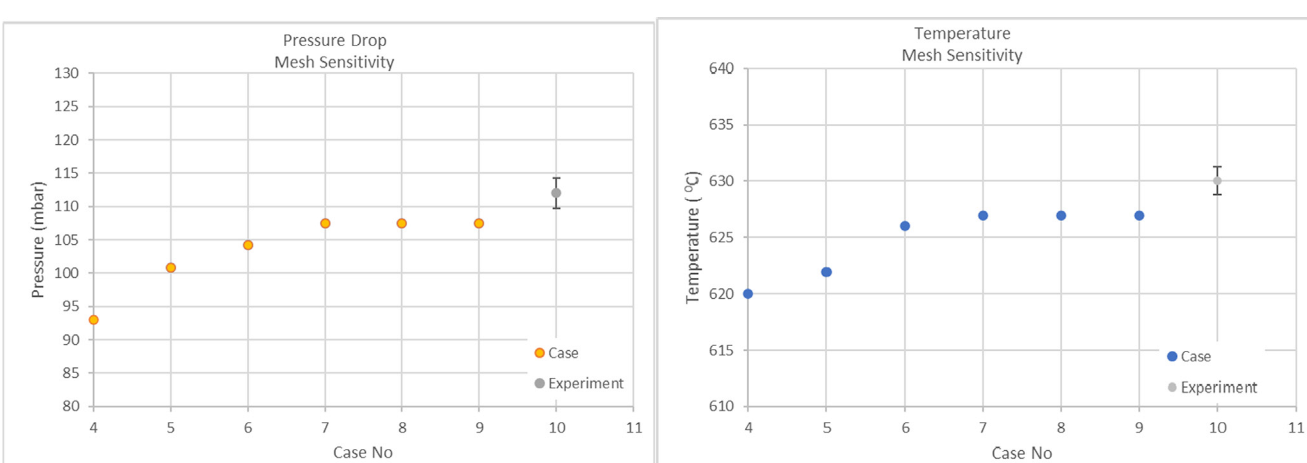

Fig. 7 Mesh Sensitivity of the Cases for Pressure Drop and Temperature.

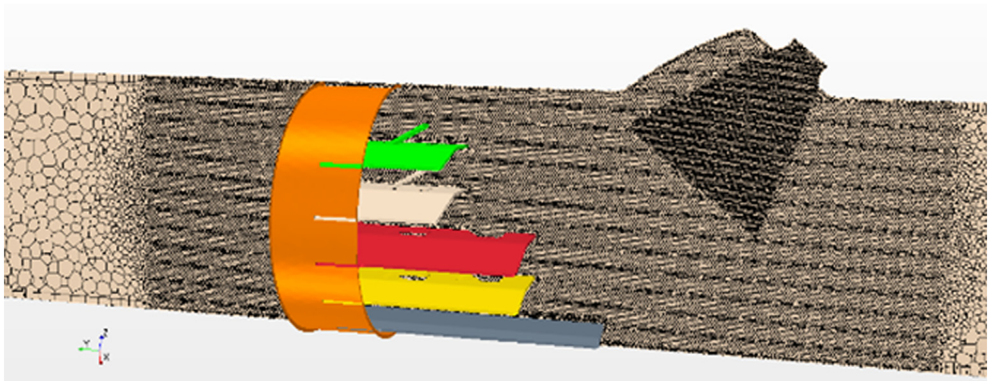

Fig. 8 The meshed of the mixer and injection region.

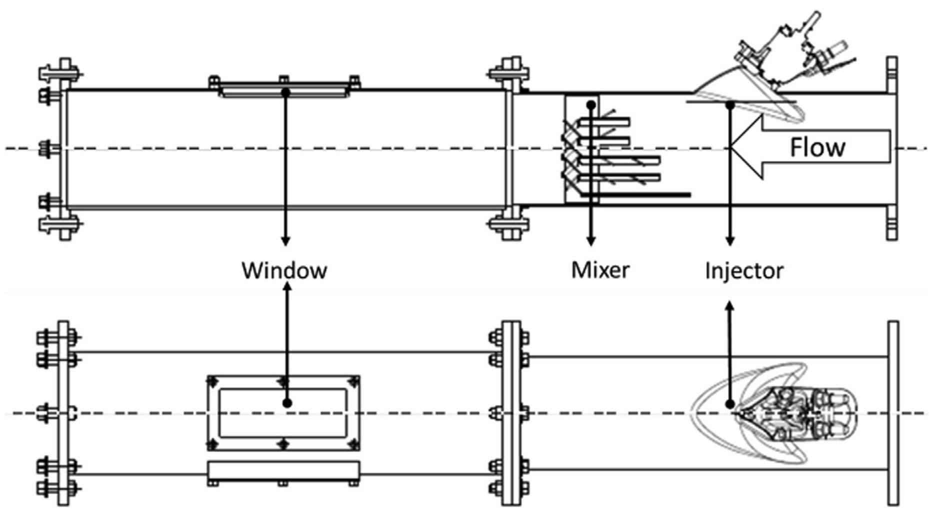

Fig. 9 PIV measurement at the pipe window.

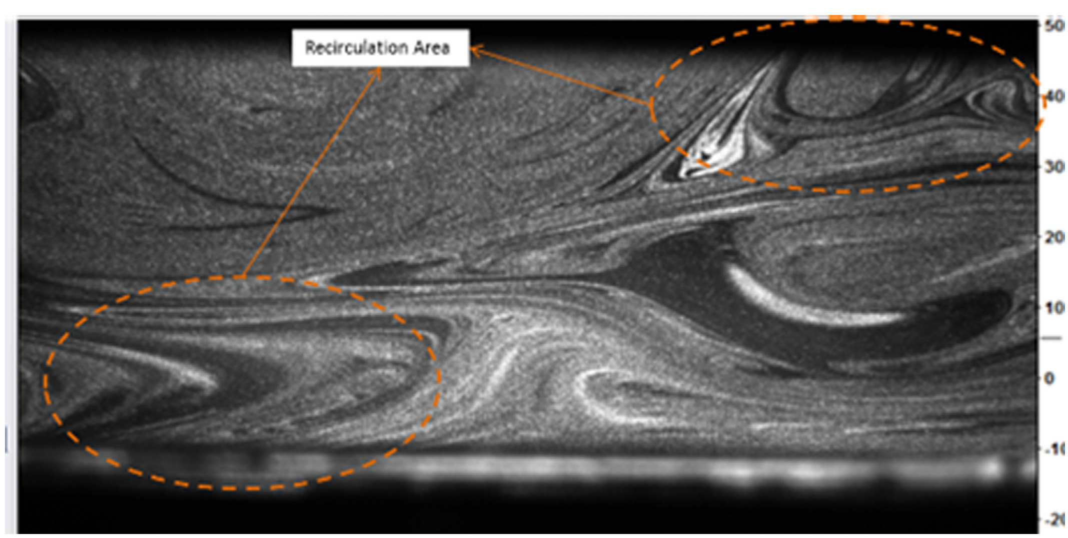

Fig. 10 Flow visualization flow field.

into the pipe wall per unit area. Therefore, the CFD results are consistent with the higher maximum injection rate without becoming wet with the higher exhaust mass flow rate.

Figs. 16 and 17 show particle trajectories colored by diameter at different time steps. Downstream of the exhaust line, some particles still contain water may be due to the relatively

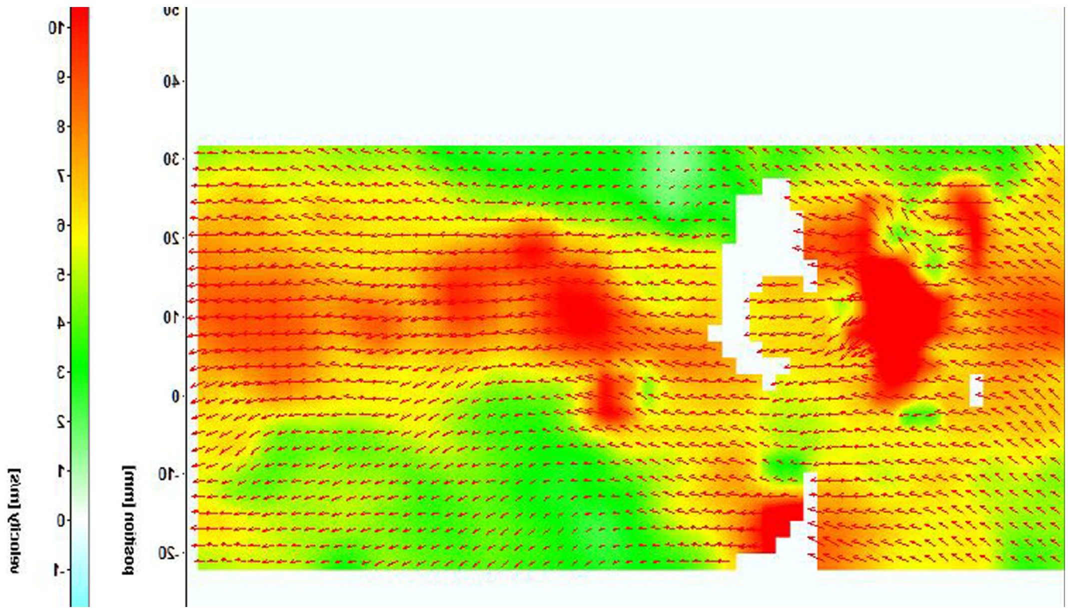

Fig. 11 Velocity vector from PIV measurement.

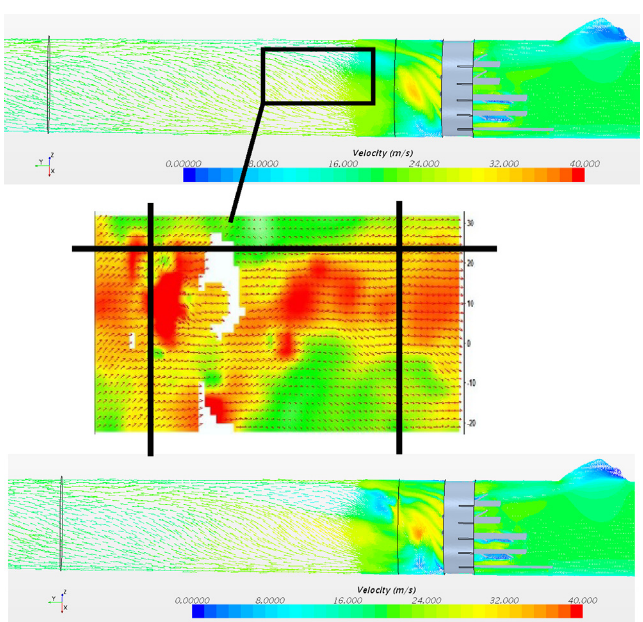

Fig. 12 Velocity vector at the cone RMS.

low gas temperature and the short residence time, related to the distance between the injector and the monolith reactor. Fig. 16 shows the diameter of aqueous urea in droplets. The aqueous urea diameter decreases due to this shape decomposition. In addition, due to the incomplete separation, there are many droplets with high mass aqueous urea fraction, especially near the SCR monolith.

The effect of in-tube mixing devices, usually downstream of the injector, with mixers installed on the inner tube wall, promotes droplet evaporation, disintegration, and distribution of the spray. The mixer has a significant influence on the disintegration process. Fig. 18 shows the application of the mixer.

The results below show the droplet distribution with the exhaust aftertreatment system for different time steps.

Results were plotted in the time step when the urea dosage reached the peak in face selection. Fig. 19 shows the results of urea injection.

It appears that the particles can reach the SCR catalyst without entirely decomposing. According to Fig. 19. Droplets reaching the SCR monolith contain approximately 68.8% aqueous urea, meaning less than 31.2% of aqueous urea is separated during the exhaust line transition. Gas temperature and short residence time are the main reasons for this decomposition. One way to ensure successful evaporation and separation is to add a urea mixer to the practical exhaust line. However, under low-temperature conditions, undesirable deposits may form on the blades of the mixer.

Fig. 20 shows the droplet diameter upstream and downstream of the mixer. This result shows us the efficiency of the mixer in terms of the droplet disintegration process. The flow cannot break up the spray particles at such a reduction. This mixer provided a 50% reduction in the size of the droplets. The droplets' momentum is subtracted from the CFD results to compare mixer performance. High droplet velocity with large droplet size improves mixing performance, but lower droplet velocity with small droplet size reduces mixing performance. Therefore, the momentum of the droplets provides practical information for comparing mixer performance (see Fig. 21).

Therefore, ammonia is produced from these droplets closer to the SCR monolith. As a result, greater ammonia concentration is observed near the SCR monolith in the mixer use application.

Mixer Performance Criteria = SMD Average of the Upstream Mixer / SMD Average of the Downstream Mixer

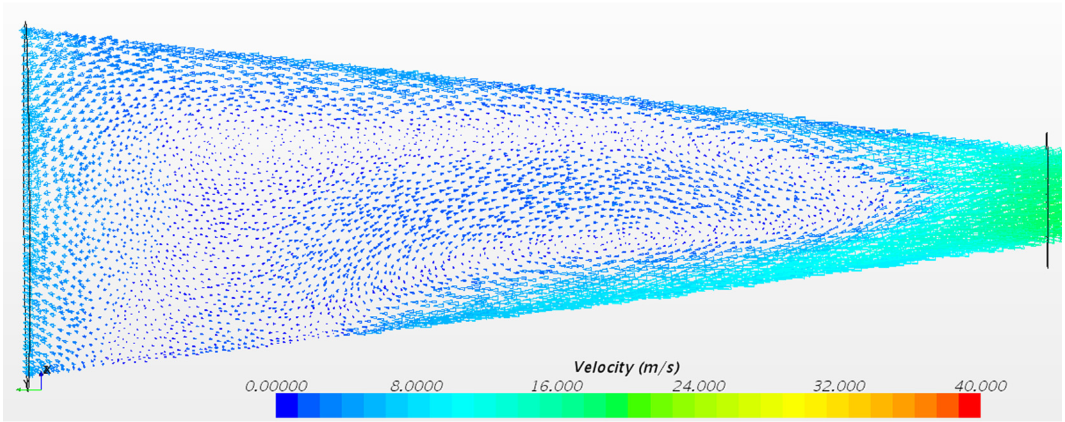

Fig. 13 Velocity vector distribution for the k-epsilon model.

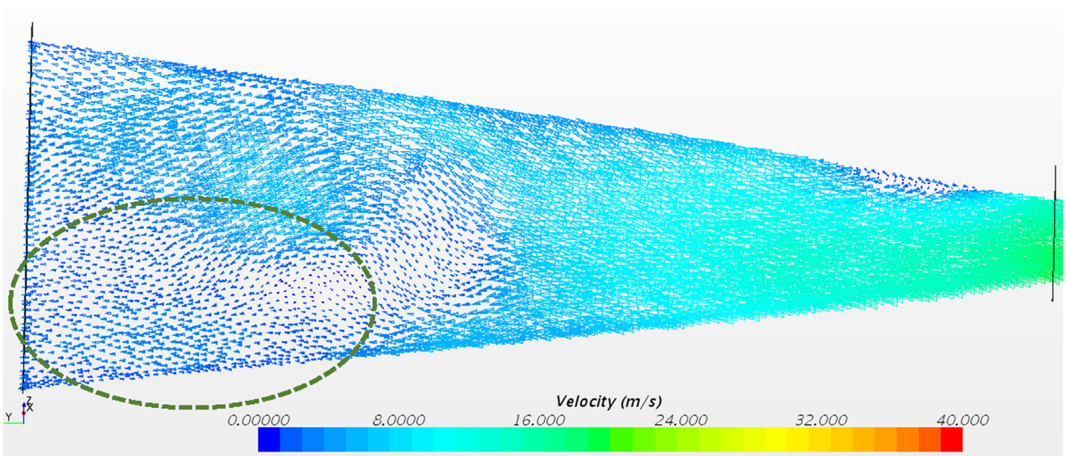

Fig. 14 Velocity vector distribution at the cone for the RSM model.

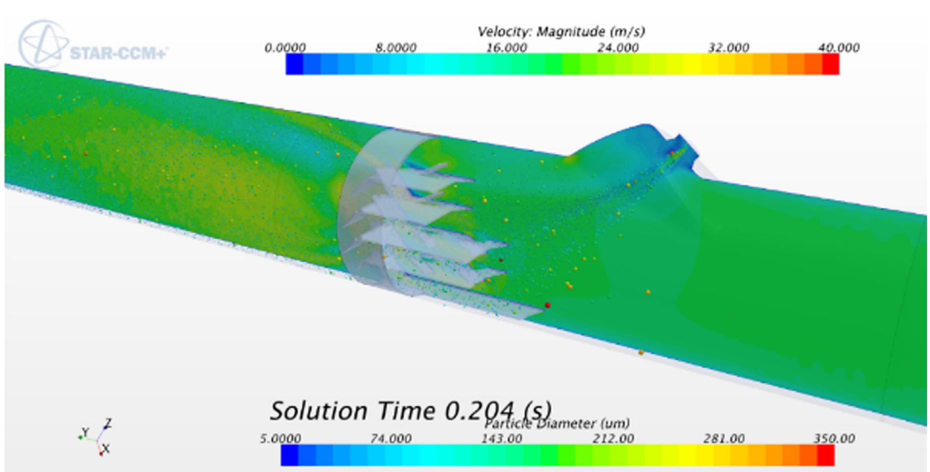

Fig. 15 Droplet Distribution into the system.

Plate mixer type's mixer performance criteria are 0,45. Spray penetration length is three diameters of the pipe.

Vane type mixer breaks up the droplets; hence the droplets evaporate rapidly. After mixer performance investigation, vane type mixer performance criteria is 0,25. This type of mixer has a more powerful breakup performance than the plate-type mixer. Spray penetration length is 1.5 in diameter of the pipe. Spay penetration is one of the parameters to show the mixer's efficiency.

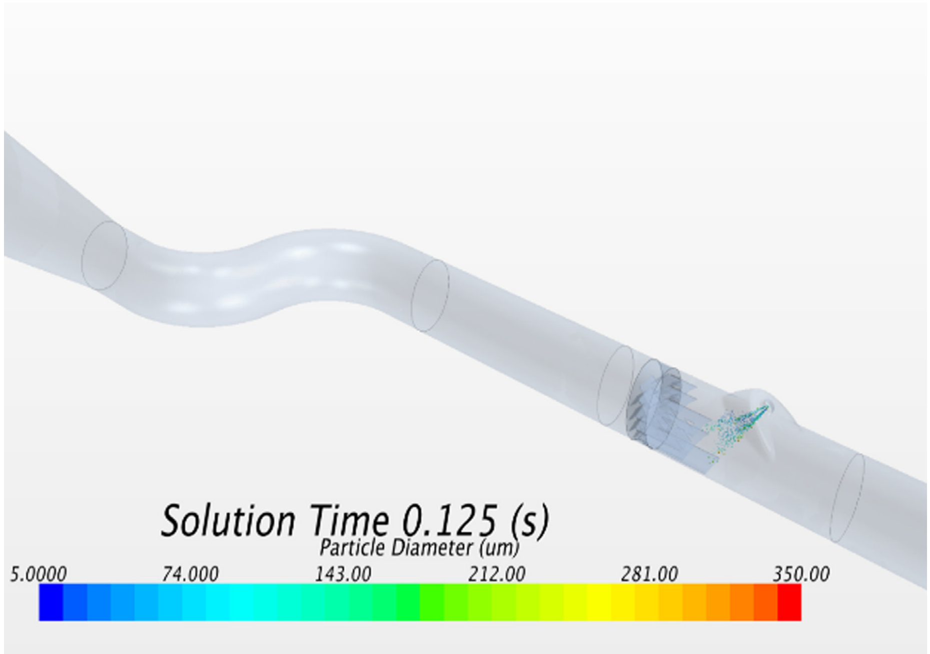

Fig. 16 Droplet Distribution across the system at 0.125 s.

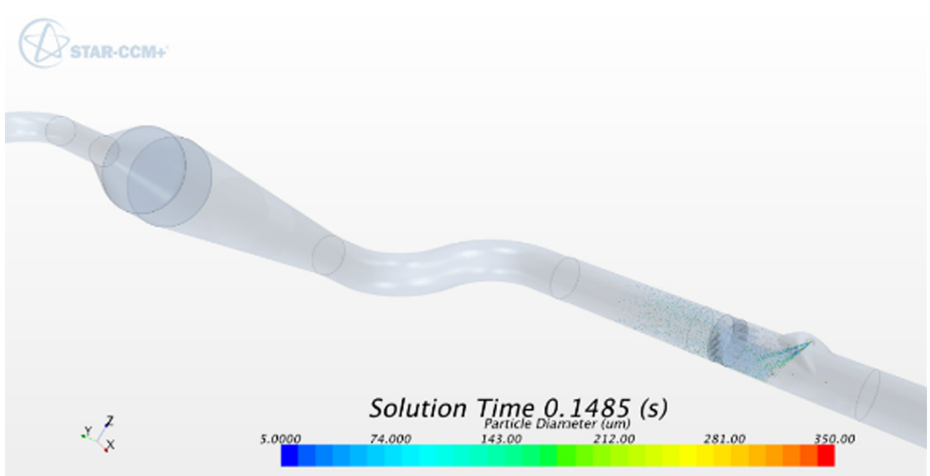

Fig. 17 Droplet Distribution across the system at 0.1485 s.

5. Conclusion

This study investigated UWS injection and evaporation in hot air flows in transparent glass ducts and under conditions similar to diesel exhaust systems. Promising optical techniques have been used to obtain information about the channel wall's liquid film formation under different operating conditions where air mass flow rate, temperature, and injection rate vary.

Multi-component UWS injection modeling and multi-reaction modeling as thermolysis and hydrolysis have been applied to the sequential exhaust aftertreatment system and validated with flow test bench capabilities such as pressure, temperature NOx and FTIR information. PIV gives an excellent result for correlating this complex SCR system.

Numerical simulations developed for droplets and species show the SCR system's dependence on injection properties and flow field parameters. The perfect fit has been demonstrated in the injection and flow areas between the numerical and flow test bench.

The following conclusions can be drawn from this study.

In this study, it was observed that the Reynolds strain was sufficient to model the turbulence model. To directly validate the turbulent exhaust flow field and spray simulation, PIV measurement and RSM simulations may be employed. The heat transfer correlation study of the inline exhaust aftertreatment system shows that conjugate heat transfer is required.

Mixers are quite effective in reducing deposits in addition to serving their primary purpose of enhancing mixing between

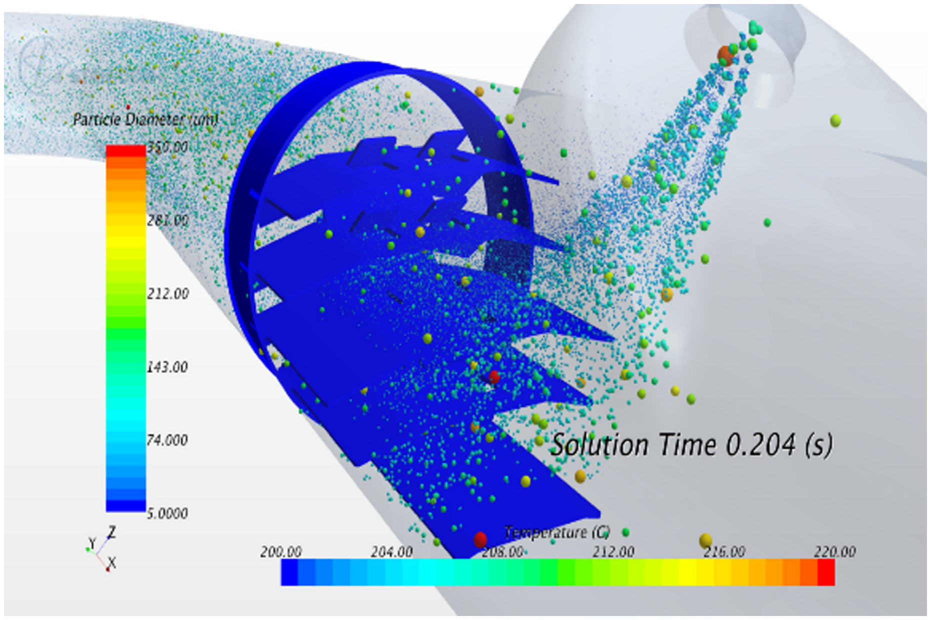

Fig. 18 Droplet distribution through the mixer at 0.204 s.

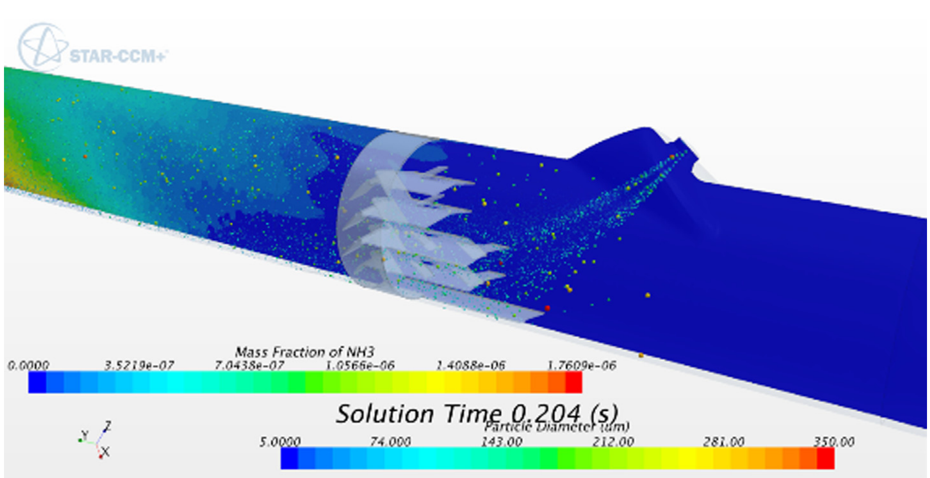

Fig. 19 Droplet distribution along with the system for time 0.01 s.

exhaust gas and spray. Heat transfer by spraying on the mixer's hot surfaces results in improved boiling and convective heat flow. Mixers with a significant surface area promise to increase conjugate heat transfer, but agitators often reduce the spray particle transport length. Mie scatter and PIV measurements of an SCR spray under conditions representative of diesel engine exhaust gas were obtained in an optically accessible flow test rig. This comprehensive data set was also used to validate a numerical platform for SCR spray simulation. Combining experimental data and other results obtained by the validated model allows a better understanding of the spray mixing dynamics found in SCR exhaust gas aftertreatment systems. The validated model is beneficial for SCR spray pattern optimization, and more validation data is required regarding the vapor phase in the downstream position.

The higher gas flow rate's direct result is the increase in droplet entrainment and is significant for droplets smaller than 50 μm. On the contrary, the effect on larger droplets is much less pronounced. These tiny droplets may not reach the channel's lower planes or show significantly shallower flow angles (i.e., aligned to flow). The largest droplets show a gradual transition from the initial injection angle to the flow direction. The first result is to reduce the spray density in higher flow situations while the spray is spread over a wider area. Respectively, so is the wall-soaking zone. The reduction in density was shown to be up to 50%. However, most of the spray mass still strikes, but the potential film formation is significantly reduced.

The performance of the vane-type mixer and plate-type mixer were investigated and compared to validate this methodology. The mixer performance criteria show that the vane type mixer has better performance than the plate type mixer. In addition, spay penetration length gives the same results.

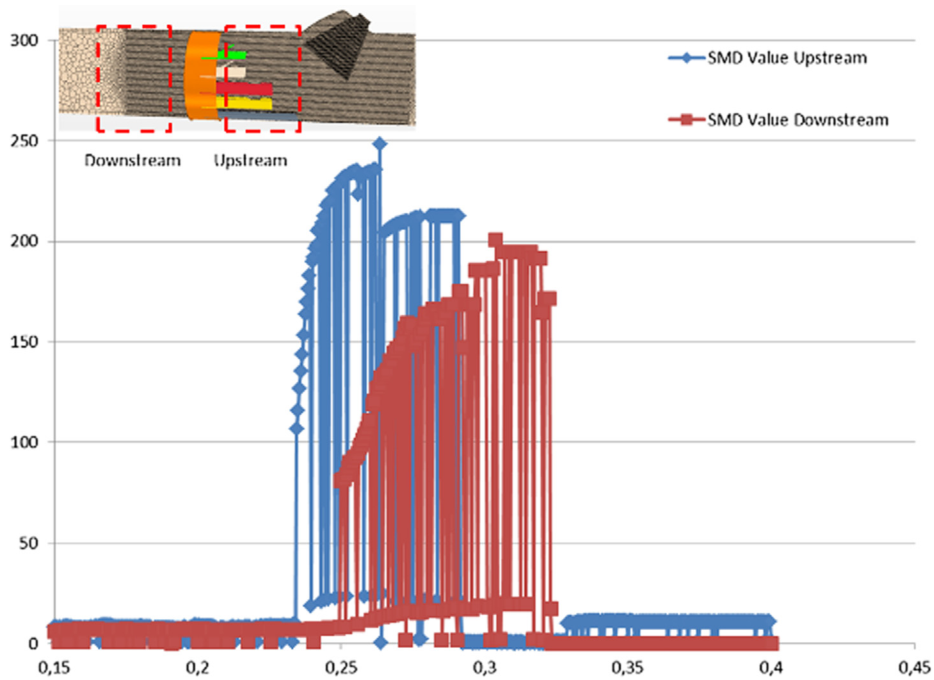

Fig. 20 SMD Value for Upstream and Downstream of the Mixer.

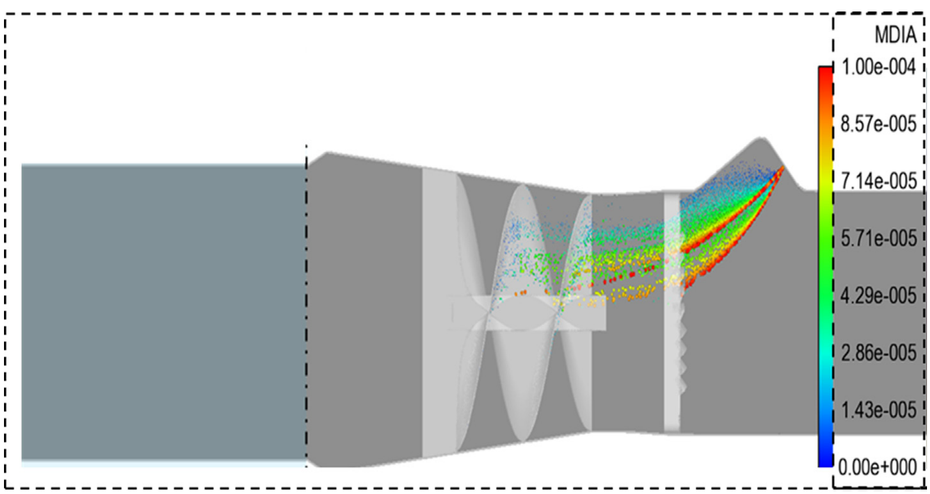

Fig. 21 Vane Type Mixer.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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