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Experimental and numerical assessment of impingement and mixing of urea–water sprays for nitric oxide reduction in Diesel exhaust ☆

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HIGHLIGHTS

- Experimental and numerical evaluation of SCR sprays in cross-flows.
- Mie scattering and Phase Doppler Anemometry data to study spray density and droplet diameters respectively.
- Kidney vortices are present only in low cross-flow velocities and improve mixing.
- High vapor concentration near the floor in high cross-flow velocities and near the side-walls in low cross-flow velocities.

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ABSTRACT

This study presents a joint experimental and numerical investigation of a spray used in selective catalytic NOx reduction (SCR) after-treatment systems for Diesel engine exhaust gases. The focus lies on the impingement conditions and distribution and mixing mechanisms of the spray in cross-flowing exhaust gases. These aspects are vital to system performance but still not well described.

A pressure-driven SCR injector is characterized in an optically accessible flow test rig at different temperatures and mass flow rates representative of Diesel engine exhaust gas conditions by means of Mie scattering and Phase Doppler Anemometry (PDA). The effects of cross-flow velocity and temperature on spray structure, droplet size and velocity distributions are assessed resulting in a comprehensive characterization of the spray. Results show that the dense spray core, with droplets up to 200 μm, only moderately reduces in density as smaller droplets are entrained at high exhaust flows. Wall impingement conditions however vary substantially as impingement angles are shallower at higher cross-flow velocities.

A detailed assessment of the numerical model is presented and validation is carried out at different measurement locations of interest. The predicted droplet size distributions and velocities follow the observed trends and impingement angles as well as spray film areas on the channel floor are also in agreement with the experimental data. The validated model is subsequently used to numerically study the mixing dynamics.

The findings suggest that at low cross-flow conditions two counter-rotating kidney vortices are formed which entrain reflected droplets of the spray impinging on the channel floor, which leads to improved mixing. Vapor concentrations increase close to the side walls and reflected droplets lead to film-formation on the side walls. At higher cross-flow velocities, vortex formation is not evident and spray-wall interaction is less pronounced – impairing mixing and leading to a reduction in concentration uniformity at down-stream locations. Film formation and high vapor concentrations are restricted to the bottom channel centerline.

1. Introduction

Due to their unrivalled efficiency, Diesel engines are widely used in on- and off-road heavy-duty application, power generation as well as passenger and freight transport. The nature of the energy

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Nomenclature

CFD	computational fluid dynamics	U_o	free stream air velocity
SCR	Selective Catalytic Reduction	U_{spray}	spray velocity
PIV	particle image velocimetry	Cdf (d)	fraction of the total volume occupied by droplets of diameter less than 'd'
PDA	Phase Doppler Anemometry	d_o	Rosin Rammler scale parameter
SMD	sauter mean diameter	k	Rosin Rammler shape parameter
RNG	re-normalization group turbulence model	RR	Rosin-Rammler
RANS	Reynolds Averaged Navier Stokes	u,v,w	velocity components along x, y and z-axes respectively
d_{noz}	nozzle orifice diameter	x_s	x-coordinates with respect to spray axis
T	free stream air temperature		
ρ_o	free stream air density		

conversion process encompassing a wide range of equivalence ratios leads to harmful emissions, viz. NOx and soot. For the abatement of the former, different techniques are in use to meet current and forthcoming legislations: On the one hand, in-cylinder measures are employed which aim at lowering the combustion temperature, see e.g. [1,2] and references therein. The second widely adopted approach uses Selective Catalytic Reduction (SCR) of the exhaust gas stream by means of ammonia as a reducing agent over Vanadia or Zeolite based catalysts. While lower engine temperatures due to in-cylinder techniques may reduce NOx emission at the source, they also reduce engine efficiency. The latter approach therefore has an inherent thermodynamic advantage.

While modeling of the catalytic channels is at a relatively mature level cf. e.g. [3,4], the processes leading to the availability of NH_3 at the catalyst entrance are considerably less well studied. These encompass the injection of a urea–water solution in a cross-flow configuration, as well as thermolysis and hydrolysis reactions taking place in the hot gas consequently providing the reducing agent. As Diesel engines are operated over a broad range of loads and engine speeds, conditions in the exhaust stream vary considerably in terms of pressure and temperature levels as well as mass flow rates. Aside the requirements of high ammonia uniformity at the catalyst entry, especially at low temperatures [5], optimal dosage for minimal ammonia slip over the entire engine operating map must be ensured. SCR injection systems must further avoid deposit formation in the after-treatment system [6–10] which may lead to reduced conversion efficiency or finally malfunction of the system. Many studies on the topic of overall SCR performance under various conditions rely on theoretical and numerical modeling and analysis.

A large number of studies of sprays in cross-flow conditions can be found, but these do not specifically consider conditions relevant to SCR applications. Possible mixing effects occurring have been discussed in studies focused on atomization and sprays; but these have yet to be applied to SCR sprays in particular. Ref. [11] report the formation of roll-up vortices and their attenuation in a cross-flow channel for low-pressure gasoline sprays. Wall impingement and film stripping have also previously been discussed in detail [12,13]. Flow conditions significantly affect spray structure and mixing, which are of vital importance to SCR performance.

Most SCR studies focus on the dependence of conversion performance on global uniformity and flow conditions, without discussing the underlying mixing processes. Only few studies on SCR sprays in the presence of cross-flow are documented in the literature [14–21] and further understanding is crucial for further improvement of SCR injectors in view of stringent emission legislations.

Although the aforementioned staple SCR-spray studies [14–18] concerned themselves with urea-SCR injection to investigate overall SCR mixing performance, they specifically refer to the limited experimental data on the topic. Data was either explicitly not available [16], reliant on few sources or was gathered specifically for the given case [14,18]. Furthermore, the fundamental aspects of the impingement and mixing processes are not discussed. The conditions considered do not cover an extensive range of Diesel exhaust conditions and omit the most problematic cases at low temperatures and gas flows. The variety of SCR injectors in use today, which may behave very differently, further complicates the issue.

Newer studies still rely heavily on experimental data gathered in the before-mentioned instances and only recently data has been available on entrainment, mixing, evaporation and impingement [19,22,23]. The study presented in [19] experimentally investigated spray density across a wide range of conditions, while in [22,24] droplet evaporation has been studied.

The goal of this study is hence threefold, namely (I) the procurement of experimental data for sprays from an SCR injector in an optically accessible test rig operated at Diesel exhaust gas typical conditions, (II) further validation of a numerical platform for SCR sprays by means of the acquired data and (III) to carry out an in depth analysis of the experimental data and to exercise the model towards improved understanding of mixing and impingement dynamics occurring in SCR sprays in cross-flow.

2. Experimental setup

Experiments were conducted on the EMPA high temperature flow laboratory described in more detail by Spiteri et al. [19]. The test rig preconditions a mass flow of dry air to a given temperature to emulate exhaust flow relevant to different Diesel engine operating conditions. A commercial six-hole disk-type urea injector with a nozzle orifice diameter of 210 μm was installed at an inclination angle of 50° with respect to the flow direction resulting in a spray in cross-flow configuration; a schematic of the test rig and injection location is shown in Fig. 1. Spiteri et al. [19] state, that during operation at 9 bar liquid pressure also used for this study, the sprays from the individual nozzle holes merged into one conical spray with negligible indication of multi-hole injection in the downstream spray pattern. Fig. 1 also shows the location of optical measurement techniques employed to investigate the spray. Water has been used to represent urea–water-solution (UWS) based on findings from [19] reporting that this simplification is able to replicate the atomization dynamics of SCR system very well, while avoiding complications caused by deposit formation during experiments. The latter is especially important to ensure reliable optical access.

For planar laser sheet Mie scattering, two 4 ns laser pulses at 532 nm were generated 25 μs apart. The laser sheet horizontally traverses the channel at the locations specified in Fig. 1 – the observable region is however limited by the upper window size. A top camera positioned perpendicularly to the laser sheet