Joint experimental and numerical study to evaluate the effect of injection pressure on SCR system performance

Ł.J. Kapusta*, R. Rogóż, D. Bojanowski
Warsaw University of Technology, Faculty of Power and Aeronautical Engineering, Institute of Heat Engineering, Nowowiejska 21/25, Warsaw, 00-665, Poland
*Corresponding author: lukasz.kapusta@pw.edu.pl

Introduction

SCR (selective catalytic reduction) systems are widely used in power generation and automotive sectors. So far, the largest market for SCR systems has been related to automotive compression ignition (CI) engines. Ongoing electrification is expected to slowly limit that market. Among the engine applications for SCR technology which are expected to grow in the future are stationary and marine CI and dual-fuel engines, as well as stationary lean-burn spark ignition gas engines intended to work in areas of extremely low emission limits. When equipped with an SCR system the engine then can be optimized to maximum efficiency, since NOx are reduced in the aftertreatment system. Another potential market is related to increased interest in ammonia combustion which leads to high NOx emissions. Regardless of the application, the principle is the same, and the crucial element to achieve efficient NOx reduction is to properly distribute a urea-water solution (UWS) over the exhaust gas stream, evaporate the water, convert the urea into ammonia and mix it with exhaust gases before it reaches the inlet to the catalyst. This process is strongly dependent on the spray and its parameters need to be properly adjusted to a specific exhaust system's design.

In this study we have demonstrated the research procedure based on coupled experimental spray research and CFD (computational fluid dynamics) simulations, to evaluate the injection pressure's influence on an SCR system's performance; while avoiding the time consuming and expensive iterative process of manufacturing and testing several series of prototypes. The method presented here is a universal method to limit experimental research and speed up the development process of devices employing liquid injection; it can be applied to fuel injection as well. In order to limit the computational time, the simulations presented here were conducted on a small-scale SCR unit designed for an automotive CI engine and constitute prerequisites for large-bore stationary engine simulations.

The presented research was conducted for two injection pressures, namely 0.4 and 0.5 MPa (gauge pressure), and was to determine whether its decrease from 0.5 to 0.4 MPa leads to a considerable change in the UWS-exhaust gas mixing performance. The mixing quality was evaluated using CFD simulations. Wall film formation and the uniformity of the ammonia concentration were used to quantitatively assess this process. The full exhaust system simulations needed to be preceded by some UWS spray experimental research, to determine the spray properties at the considered injection pressures. In this study the required data was taken from the literature [1]. The experimental data was used as input parameters to CFD calculations and to calibrate the spray models. The CFD simulations were performed for three different operating points with different exhaust gas mass flow rates.

Material and methods

The simulations were performed on an SCR model for a small automotive CI engine. The model included the SCRF (selected catalytic reduction on filter), a DOC (diesel oxidation catalyst) as well as a mixer and an injector mounted between the catalysts (Figure 1). As seen in Figure 1 the UWS was injected towards the static mixing device. The computational mesh was constructed starting from the catalysts' connector, where the polyhedral mesh was built. The end planes of the connector (outlet from the DOC and inlet to the SCRF) were then swept to create structural meshes in the catalysts' bricks. The mesh was created using AVL FIRE M™ v.2018 software.

The CFD (computational fluid dynamics) simulations were performed on the AVL FIRE™ v.2014.2 software using the RANS (Reynolds-averaged Navier-Stokes) method. The turbulences were modelled according to the k-ζ-f model [2]. The DOC and SCRF were modelled as one-direction porous zones, where the pressure drop was calculated by the Forchheimer formula [3].

For spray modelling, the Lagrangian approach was employed. The parameters used to properly represent the spray such as: the initial jet velocity, spray plume angle, injected mass, and the droplet size distribution were taken from the experimental research in the literature. The UWS decomposition was modelled as a 2-step process; where first, water evaporates from the droplets until only urea remains, and then the urea decomposes into NH_3 and HNCO in a thermolysis process [4]. The droplet-wall interaction was modelled according to the Kuhnke approach [5].

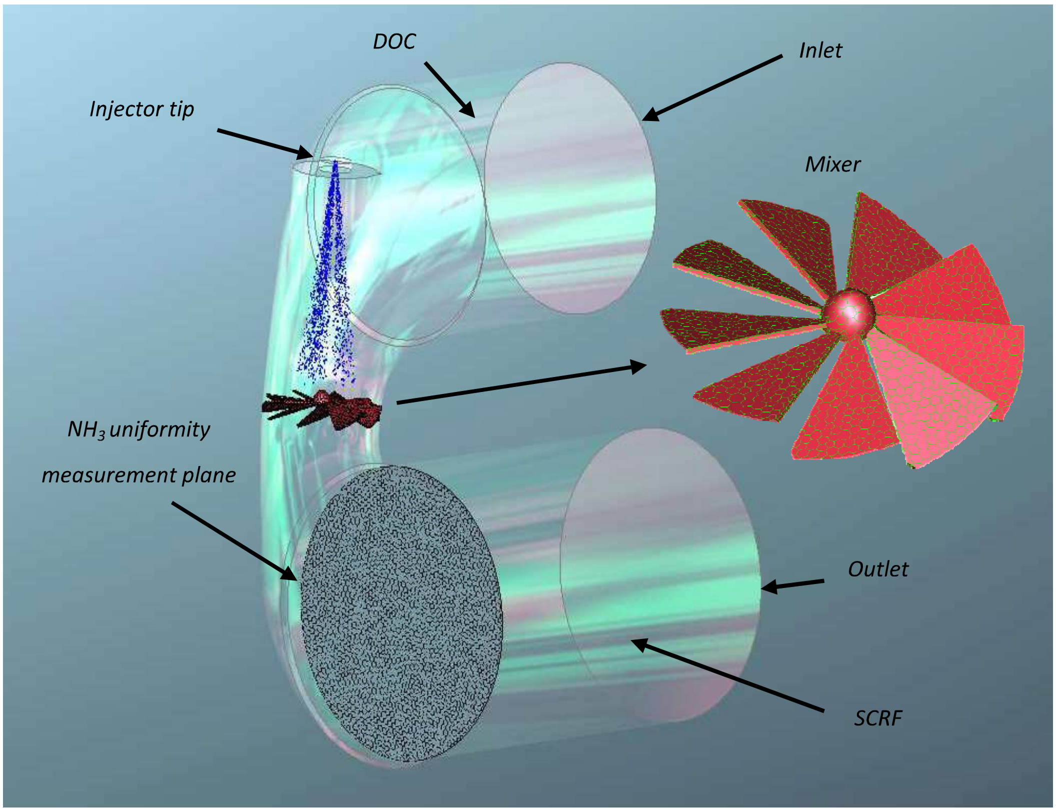

Figure 1. Geometrical model of the SCR system

The simulations were performed for two different injection pressures. This required two different simulation set-ups since most of the spray parameters used to model the spray such as: the initial jet velocity, spray plume angle, injected mass, and the droplet size distribution, were different. The spray model parameters were taken from the literature [1] and are shown in Table 1.

Table 1. Spray model parameters (based on [1])

Parameter	Unit	p_{inj} = 0.4 MPa	p_{inj} = 0.5 MPa
Inclination angle	deg	6	6
Single plume angle	deg	4.9	7.3
Static volumetric flow	cm^3/s	0.74	0.82
Initial jet velocity	m/s	24.5	26.1

The simulations were performed for three different exhaust gas mass flow rates, which required different injection durations. The simulation parameters for the three mass flow rates and two injection pressures are shown in Table 2.

Table 2. Simulation parameters

Exhaust gas mass flow kg/h	Exhaust gas temperature °C	NOx concentration ppm	UWS dosage mg/s	Injection duration p_{inj} = 0.4 MPa ms	Injection duration p_{inj} = 0.5 MPa ms
100			17.74	5.5	5.0
200	300	200	35.49	11.1	10.0
300			53.23	16.6	15.0

Results

The ammonia concentration distribution at the plane 12 mm downstream from the SCRF inlet is shown in Figure 2. As a quantitative parameter for evaluation of the uniformity of the ammonia distribution, the time-averaged ammonia mass uniformity index *UI*, was calculated. The calculated values of the ammonia uniformity index are shown together with the ammonia concentration contours in Figure 2.

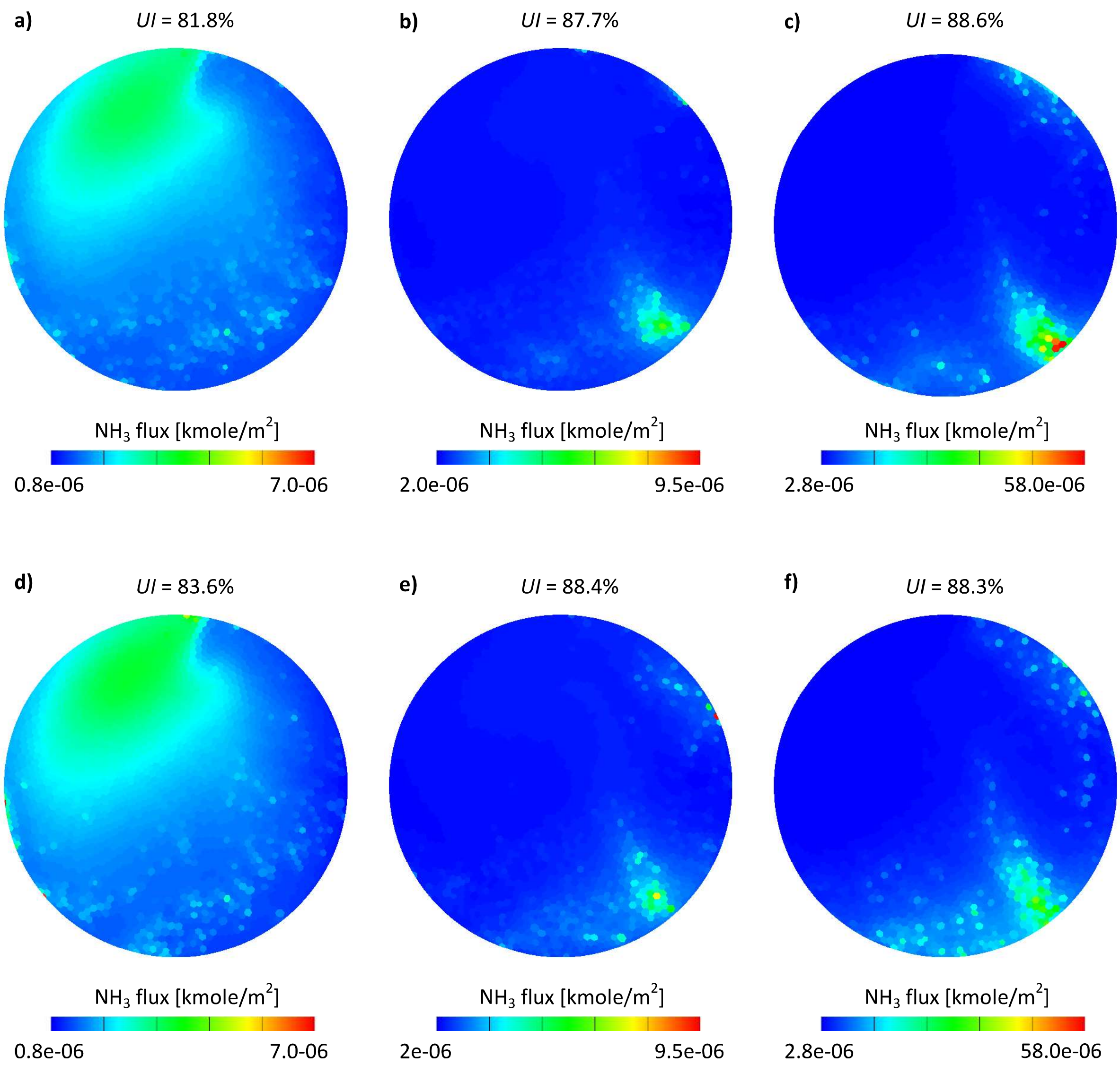

Figure 2. Time integrated NH3 molar flux scaled to the cell face area - 12 mm from the SCRF inlet for different exhaust gas mass flow conditions and injection pressures: (a) 100 kg/h, p_{inj} = 0.4 MPa; (b) 200 kg/h, p_{inj} = 0.4 MPa; (c) 300 kg/h, p_{inj} = 0.4 MPa; (d) 100 kg/h, p_{inj} = 0.5 MPa ; (e) 200 kg/h, p_{inj} = 0.5 MPa; (f) 300 kg/h, p_{inj} = 0.5 MPa

As shown in Figure 2 the ammonia distribution is in general similar for both studied injection pressures. For low and medium mass flow rates the uniformity index was higher for 0.5 MPa injection pressure; while for the highest mass flow rate the effect was opposite; however, the difference was then negligible.

As for the wall film formation, the difference between the two injection pressures was more visible (Figure 3). The wall film mass per unit area in the case of the 0.4 MPa injection pressure was higher for all mass flow rates.

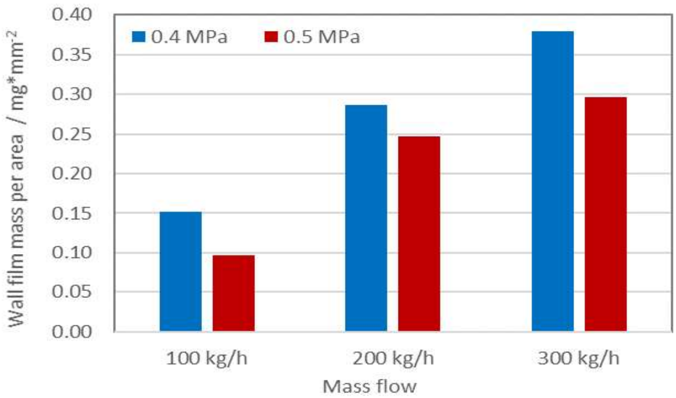

Figure 3. Wall film at the end of simulation per wetted area

Summary and Conclusions

In this study the research procedure based on the coupling of experimental spray research and CFD simulations has been used to evaluate injection pressure influence on an SCR system's performance as an alternative to the time consuming and expensive iterative process of manufacturing and testing several series of prototypes.

The contours of the ammonia concentration were in general very similar; however, differences in the uniformity index could be noticed. For the low and medium mass flow rates the uniformity index was higher for 0.5 MPa injection pressure; while for the highest mass flow rate the effect was opposite, but not as strong. It is difficult to conclude if the differences were acceptable – it depends on the design target. Although the 0.7 and 0.3 percentage point difference for medium and high mass flow seems to be negligible, 1.8 percentage point difference for the lowest mass flow rate seems to be already a considerable difference. As for the wall film formation, the differences between the two injection pressures were even more distinct. The wall film mass per unit area in the case of 0.4 MPa injection pressure was higher for all mass flow rates.

The proposed approach of linking experimental spray studies with further numerical simulations allowed the capturing of differences in the system's operation when the injection pressure was decreased. The method presented here is a universal method to limit experimental research and speed up the development process of devices employing liquid injection; it will also be applied in the simulations for a large-bore stationary engine in the future. There still remains a question about the accuracy of the simulations. This, however, can be verified for one selected design by comparing it with a single prototype test.

Nomenclature

CI	compression ignition
CFD	computational fluid dynamics
DOC	diesel oxidation catalyst
p_{inj}	injection pressure
SCR	selective catalytic reduction
SCRF	selective catalytic reduction on filter
UI	uniformity index

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