

Numerical Modelling and Experimental Characterization of a Pressure-Assisted Multi-Stream Injector for SCR Exhaust Gas After-Treatment

Achinta Varna and Konstantinos Boulouchos
Swiss Federal Institute of Tech.

Alexander Spiteri and Panayotis Dimopoulos Eggenschwiler
EMPA

Yuri M. Wright
ETH Zurich/Combustion+FlowSolutions GmbH

ABSTRACT

Simulations for a pressure-assisted multi-stream injector designed for urea-dosing in a selective catalytic reduction (SCR) exhaust gas system have been carried out and compared to measurements taken in an optically accessible high-fidelity flow test rig. The experimental data comprises four different combinations of mass flow rate and temperature for the gas stream with unchanged injection parameters for the spray. First, a parametric study is carried out to determine the importance of various spray sub-models, including atomization, spray-wall interaction, buoyancy as well as droplet coalescence. Optimal parameters are determined using experimental data for one reference operating condition. The model is subsequently applied to all operating conditions with unaltered parameters and validated by means of the measured droplet velocity fields, droplet diameter distributions and spray-tip propagations which have been characterized by means of Particle Image Velocimetry (PIV), Phase Doppler Anemometry (PDA) and shadow imaging. Finally, the model is used to investigate in detail phenomena characteristic of inclined sprays in cross-flows. Effects such as formation of vortices behind the spray core for low cross flow velocities, greater entrainment of droplets at high flow rates as well as wall film dynamics and the interaction of droplets also with the side walls are discussed in detail, highlighting the importance of the respective phenomena at the different operating conditions.

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INTRODUCTION

Sprays propagating in cross-flow conditions are encountered in many practical applications since cross-flow improves the exchange of mass, momentum and energy between liquid and gas phase. This is favorable in processes such as urea injection in SCR systems [1, 2, 3, 4, 5, 6, 7], fuel injection in turbojet/ ramjet/scramjet [8, 9, 10], spark-ignition combustion employing both Direct-Injection Stratified Charge as well as Port-Fuel injection systems [11, 12, 13], chemical sprays in agriculture sector [14, 15, 16, 17] and sprays in gas conditioning industry [18]. Consequently a wide variety of experimental studies have been conducted to understand liquid sprays in cross-flows.

An extensive experimental study specifically concerning the nature of spray under SCR operating conditions has recently been presented in [6], while experiments addressing the effect

of angle of injection are reported in [8]. Investigations have also been carried out with and without the consideration of spray-wall interaction. As shown in [9], at low weber number (We), bag-breakup of liquid jet is witnessed at low momentum ratio (q) and Rayleigh breakup occurs at high q . At intermediate We , multimode breakup is observed at low q and Rayleigh break-up happens at high q . Spray dynamics is hardly altered by q at high We . In [14] it was found that the spray region could be divided into different zones on the basis of free stream velocity, induced air speed and liquid jet velocity. Formation of vortices downstream of spray and the extent of entrainment of droplets depend on the ratio of free stream and induced air velocities [14].

The gas will entrain small droplets thus preventing them from interacting with the channel floor. Larger droplets are deflected from their original path and the impingement occurs several centimeters downwind. On the whole, droplets reaching the floor have a

much higher average diameter and velocity than they would have in the absence of cross-flow [19]. This unique feature of sprays in cross-flow enables the control of droplet size distribution actively at different locations [20]. Wall-jet vortices are formed when spray impacts the floor, which remove small droplets from the floor and introduce them into the flow [19]. However, cross-flow reduces the influence of these roll-up vortices. Increasing injection pressure reduces the effect of cross-flow. Increasing the injection timing increases film thickness and vapor layer thickness [11]. 'Splash' becomes relatively important phenomenon in the presence of cross-flows [12] and it also improves interaction between 'crowns' at the floor and droplets before impact such that the volume flux of small droplets moving from the floor increases.

The presence of a wall was found to decrease the penetration rate of the spray due to which the available impact energy is smaller than would be expected with free spray [12]. Cross-flow also helps in secondary atomization by film-stripping [13, 21]. The gas momentum promotes dispersion, partial vaporization and disruption of droplets. Cross-flow decreases normal velocity of impinging droplets. It carries away droplets more prone to deposit which leads to formation of thinner films. It also transports secondary droplets and evades their re-impact with the floor [13]. Diameters of secondary atomized droplets increase with increasing film thickness which could be achieved by reduction of cross-flow velocity or increase of fuel flow rate [22]. Film thickness increases steadily along flow direction [21].

While a broad range of experimental studies are reported in the literature as summarized above, computational fluid dynamic (CFD) studies of sprays in cross-flows are scarce. A numerical study regarding the effect of injection angle on droplet diameters and velocities is available [18]. It has also been documented that spray-wall interaction, drag force and buoyancy models are critical for sprays in urea-SCR systems [4]. [1, 2, 3, 4, 5] further reported simulations of urea-SCR systems but none of them have made detailed validation of the urea spray characteristics using extensive experiment data.

This study constitutes an attempt towards improved understanding concerning the specifics of liquid spray under SCR conditions by combining CFD and experiments. The effects of primary atomization, spray-wall interaction, buoyancy, droplet coalescence and film sub-models on the predictions have been carefully assessed. All the necessary models are optimized for one SCR condition using the available PIV, PDA and shadow imaging data. The validated set-up is subsequently validated by means of additional operating conditions. The findings are in good agreement with the fundamental characteristics of sprays in cross-flows which have been previously reported in the literature.

EXPERIMENTAL SETUP

Experimental data is gathered on a high temperature SCR flow rig [6] at the laboratory for internal combustion engines at Empa. Air of selectable mass flow is preconditioned to an adjustable temperature upstream of the rectangular injection duct. The mass flow of air is measured using hot wire anemometer. A commercially available 6-hole (orifice diameter $d_{noz}=210\text{ }\mu\text{m}$) pressure-driven disc-type injector operated at 9 bar pressure injected liquid discontinuously. Optical access to the injection site was available on all four sides. A longitudinal section of the injection site is shown in Figure 1. Shadow imaging, PIV scattering and PDA measurements were conducted. Phase-locked shadow images are made with 20 ns pulsed laser backlighting at different times during the injection cycle. 60 images are captured at each point in time, resulting in approximately 500 images for the assessment of the complete injection process at a specific exhaust flow condition. For PIV, two 4 ns pulses from Nd:YAG laser are generated with 25 μs interval. The laser sheet is formed horizontally along the channel length. Droplet PIV measurements are carried out at various vertical positions; here 786 images pairs are captured in each plane and processed to produce the mean spray velocity field by cross-correlation. Two-dimensional PDA measurements are conducted on the axis centerline $y=0\text{ mm}$ at $z=-14\text{ mm}$. PDA data on 10'000 droplets is gathered at every location for each exhaust flow condition and signal validation rates are in the vicinity of 95%. For further details, the reader is referred to [6].

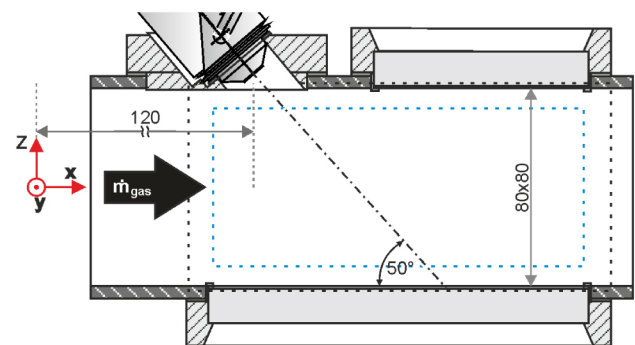


Figure 1. Cross-section through the channel axis indicating the location and orientation of the injection nozzle (injection direction along dash-dotted line), windows and coordinate system. The blue dashed rectangle indicates the window extent in the channel transversal direction normal to the viewing direction. Adapted from [6].

The air conditions which are used in this study are given in Table 1. Simulation is done without spray for 0.5 s to allow the flow field to reach steady state. Water is injected for next 60 ms with a velocity of 27.4 m/s. The injector has 6 orifices each of diameter (d_{noz}) 210 μm and temperature of injection is 293 K [6].

Table 1. Gas flow conditions used in the present work

Case name	mfr (kg/hr)	T (°C)	ρ_o (kg/m ³)	U_o (m/s)
m100t200	100	200	0.746	5.8
m100t300	100	300	0.616	7.1
m100t400	100	400	0.524	8.3
m400t300	400	300	0.616	28.2

NUMERICAL SETUP

Simulations are conducted using the commercial CFD finite volume solver STAR-CD v4.20 [23]. The computational domain is explained in Figure 2 where red line indicates the axial location of the injector. All the dimensions are in millimeters (mm). The cross section of the rectangular channel is 80*80 mm² and the length is 500 mm. According to the mesh coordinate system the geometric range extends in the three dimensions $x=[0,500]$, $y=[-40,+40]$ and $z=[-40,+40]$; where the values are in millimeters. The injector is fixed on the ceiling of the channel at an axial distance of 120 mm from the channel inlet. The spray is inclined at 50° to the flow direction (positive x-axis). The three dimensional hexahedral mesh contains around 1.1 million cells. The mesh is refined near the walls and early trajectory of spray. The volume of refined cell is 2 mm³ and that of coarse cell is 16 mm³. A grid sensitivity study has been carried out, showing that the given mesh is sufficiently well resolved. For high pressure fuel sprays, considerations put forward in [24] recommend grids with spray transversal resolutions of the order of the nozzle diameter. However, the mesh resolution used in this study was found to be sufficient, in part due to the much lower injection pressures and velocities of AdBlue dosing systems.

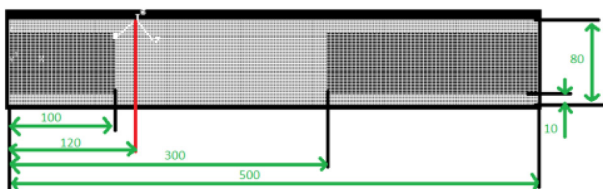


Figure 2. Mesh used in this study. Dimensions are in mm.

Standard RNG $k-\epsilon$ turbulence model is used for the Reynolds-averaged Navier-Stokes (RANS) calculations carried out in this study. 'No slip' and 'adiabatic' boundary conditions with standard wall function formulation are used. Technical air consisting of Nitrogen and Oxygen is used instead of exhaust, for non-reactive simulations. Ideal gas law, Sutherland law and polynomial c_p are used to calculate density, molecular viscosity and specific heat respectively.

Two-Phase Treatment

No significant differences were observed between water and Urea-Water-Solution (UWS) spray characteristics in a previous study [6], hence water has also been adopted in the simulations. To treat the dispersed two-phase flow a fully two-way coupled Eulerian-Lagrangian technique is used with source terms in the respective conservation equations for mass, momentum, turbulence quantities, species and energy. Evaporation is modelled based on the correlation of Ranz-Marshall; further details can be found in [23].

For droplet atomization, several models are available in STAR-CD as given in [23], which have however been developed for high-pressure injection configurations. Two different approaches have been compared in this study: 1) the so-called 'blob' model, which injects mono-disperse droplets with diameters corresponding to the orifice diameter and 2) a prescribed droplet size distribution as discussed in detail below.

A variety of droplet secondary break-up models is available in the flow field solver, cf. [23]. In agreement with the experimental findings reached in [6], the inspection of droplet Weber numbers revealed, that secondary break-up does not occur. As a consequence, no significant differences in terms of droplet diameters and velocities at different locations could be observed between the Reitz-Diwakar, Pilch-Erdman, Hsiang-Faeth and the KHRT model. As a consequence, the choice of the model for droplet secondary break-up is not important as will be discussed later.

Inter-droplet collision is treated by the model proposed by O'Rourke (hence forth referred to as the 'standard' model) which distinguishes between coalescence, separation and bouncing but only droplets located in the same cell are considered for interaction. As outlined in [23], several extensions of the original model are implemented in STAR-CD in the so-called 'advanced' collision model. These include accounting for droplet time scale effects on coalescence and collision and further make use of a cell clustering approach which enables interaction of droplets in neighbouring cells.

RESULTS AND DISCUSSION

This Section is organized as follows: first, the effects of phenomena like buoyancy, spray-wall interaction etc. on the droplet distribution are studied. Later, assessment of primary atomization models is done using experimental data. The optimized numerical set-up is used to carry out simulations for different operating conditions and the results are validated to prove the model's applicability. This spray model is subsequently exercised to study various features of inclined sprays in cross flows.

A qualitative study is conducted to examine the effects of phenomena like buoyancy, droplet-droplet collision, spray-wall interaction and wall-film as captured by STAR-CD models.