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Analyzing the Operation of a Selective Catalytic Reduction (SCR) device for NOx Reduction

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ECOFUEL · University of Southampton · Aston University · Shanghai Jiao Tong University · Aalto University · PEOPLE

Background

- Aalto University is a partner of the Ecofuel project.

- School of Chemical Technology is the biggest participant from Aalto.
- School of Engineering participates with a small contribution.

Introduction

- Nitrogen oxides ($NO + NO_2$), commonly named as **NO_x,** are harmful gases as they participate to the smog and acid rain phenomena, and to the production of ozone in lower atmosphere.
- NO_x is a typical byproduct of combustion processes, e.g. engine combustion produces NO_x .
- There are many ways to reduce NO_x emissions. Part of them reduce production of NO_x already during the combustion process, and part of them are **aftertreatment methods**, i.e. working with the NO_x already produced in the exhaust gases.

Selective catalytic reduction (SCR)

- We are studying the latter method, i.e. the aftertreatment of exhaust gases.
- Selective catalytic reduction (SCR) can be used to reduce NO_x from exhaust gases.
- In an SCR device, an urea-water solution is injected to the exhaust gases.
- The urea-water solution evaporates in the hot exhaust gases and ammonia (NH_3) is formed.
- Ammonia reacts with NO_x and transforms NO_x into harmless N_2 and water.

$$NH_3 + NO_x \rightarrow N_2 + H_2O$$

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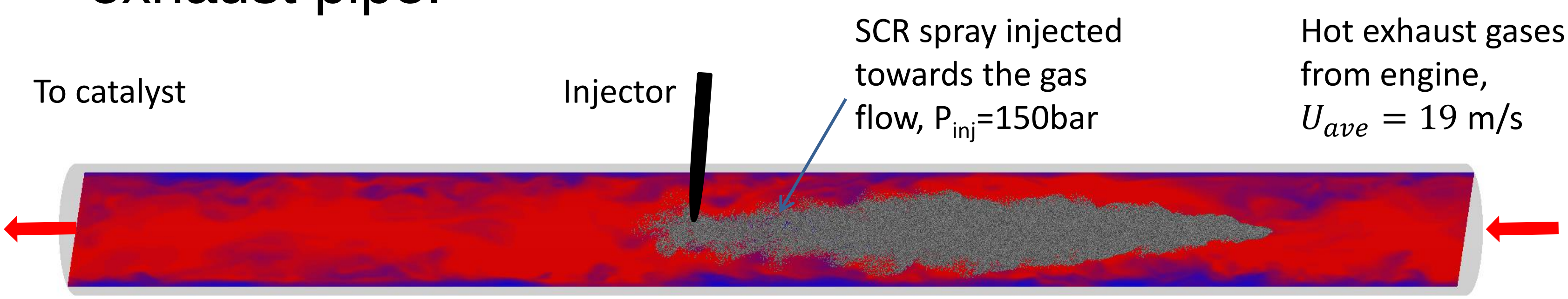
A novel SCR method

- Urea-water solution is injected to the exhaust gases with a high injection pressure (150 bar).
- Injection is directed against the hot opposing exhaust gases.
- Succesful engine experiments published in Kaario et al. 2014.
- Large Eddy Simulation (LES) method is used to capture the chaotically swirling turbulent flow in the exhaust pipe.



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Computed cases

- There seems to be very little experimental evidence from such high pressure SCR sprays, e.g. droplet sizes.
- Therefore, we will analyze four monodisperse sprays to characterize the real polydisperse SCR sprays.
- Consequently, we will use 10, 20, 30, and 40 μm droplet size sprays .

Details of the SCR spray cases.

Gas mass flow rate in the pipe [kg/h]	420
Average gas temperature in the pipe [K]	523
Pressure in the pipe [bar]	1
Average flow velocity [m/s]	19
Injection pressure [bar]	150
Injection velocity [m/s]	150
Nozzle hole diameter [mm]	0.23
Number of nozzle holes	1
Injection duration [ms]	4

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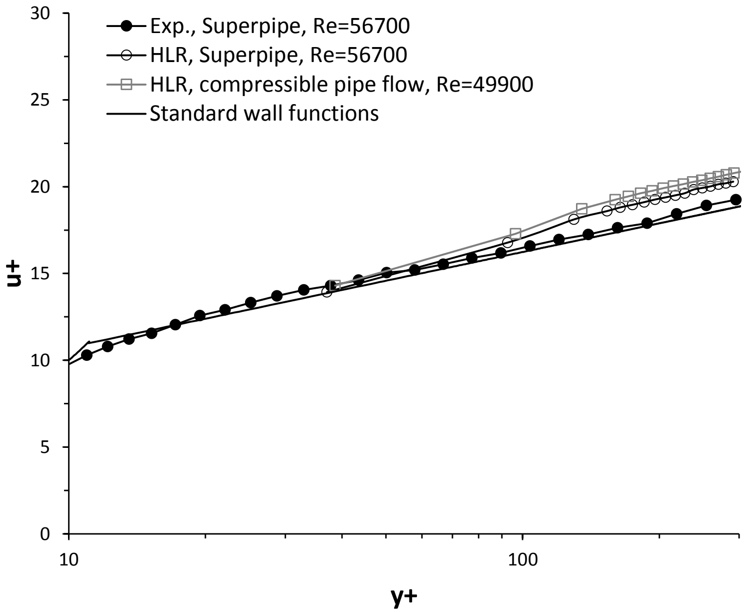
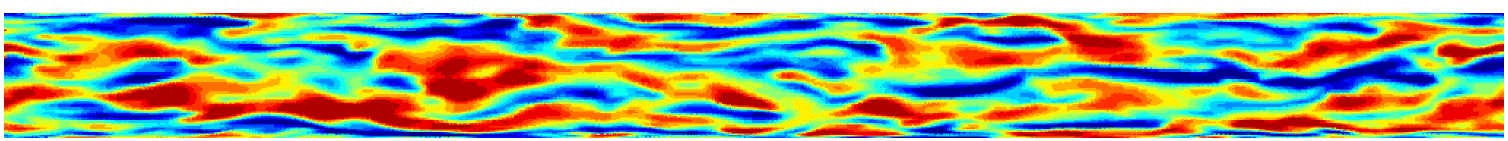
Pipe flow validation



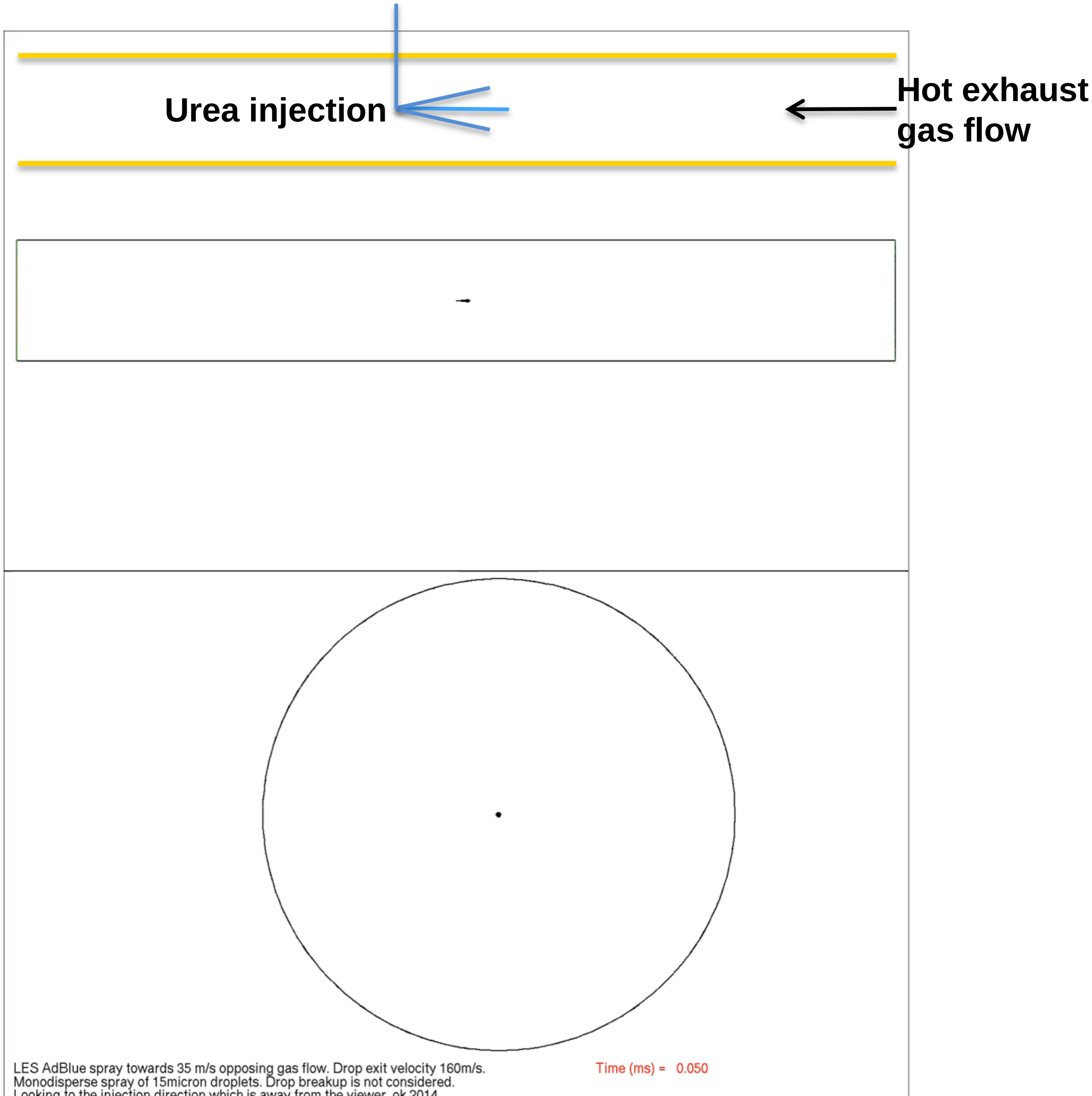
Dimensionless velocity u^+ as a function of the dimensioless distance y^+ from the wall



Axial velocity from compressible pipe flow ($\mathrm{Re} = 49{,}900$) at $y^+ = 130$. Color scale from 12 m/s (blue) to 19 m/s (red).

The dimensions of the plot is 1200 mm x 110 mm.

SCR spray mixing



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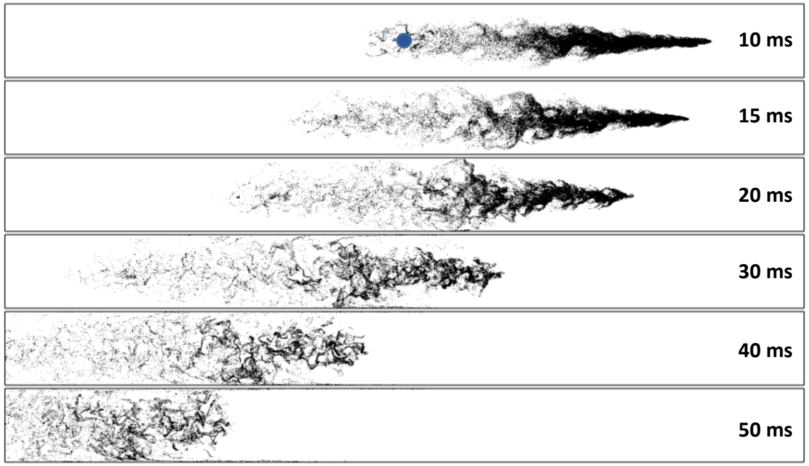
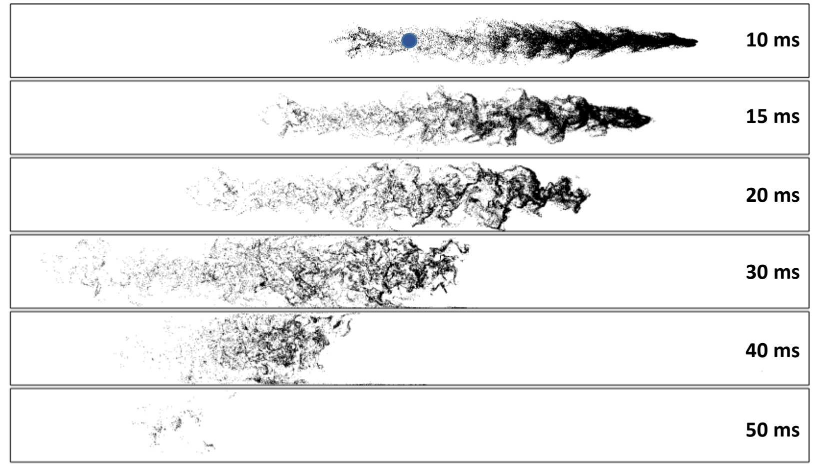
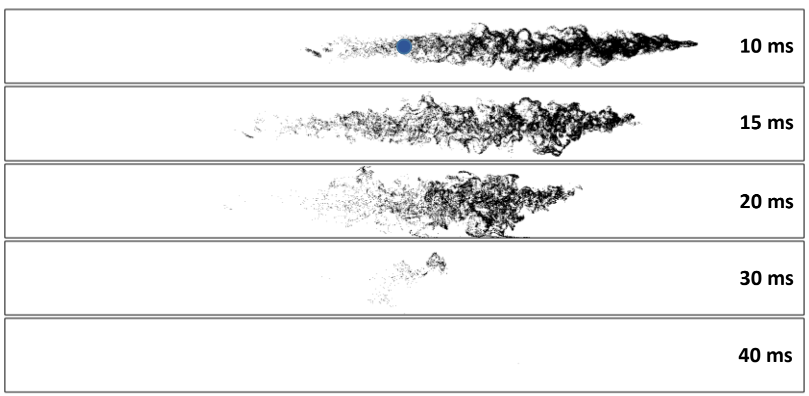
SCR spray evolution



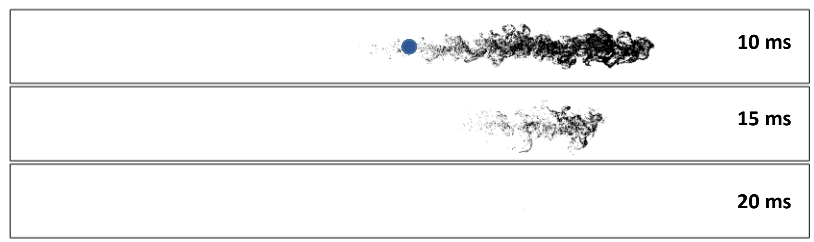
40 µm droplets



30 µm droplets



20 µm droplets



10 µm droplets

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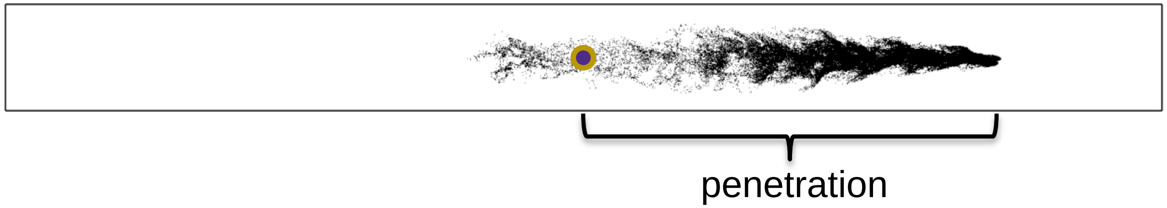
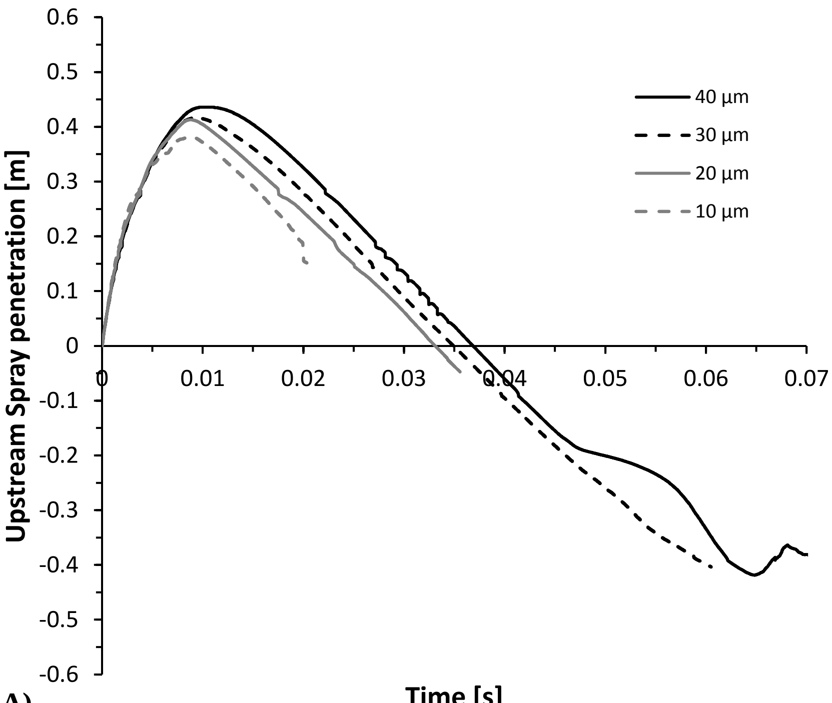
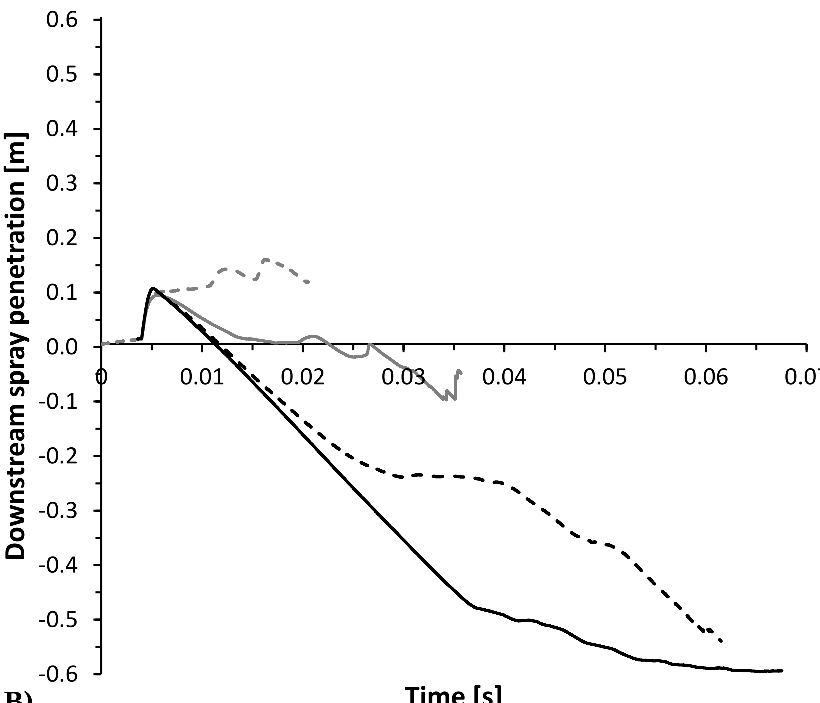
SCR spray penetration





A)

Upstream penetration



B)

Downstream penetration

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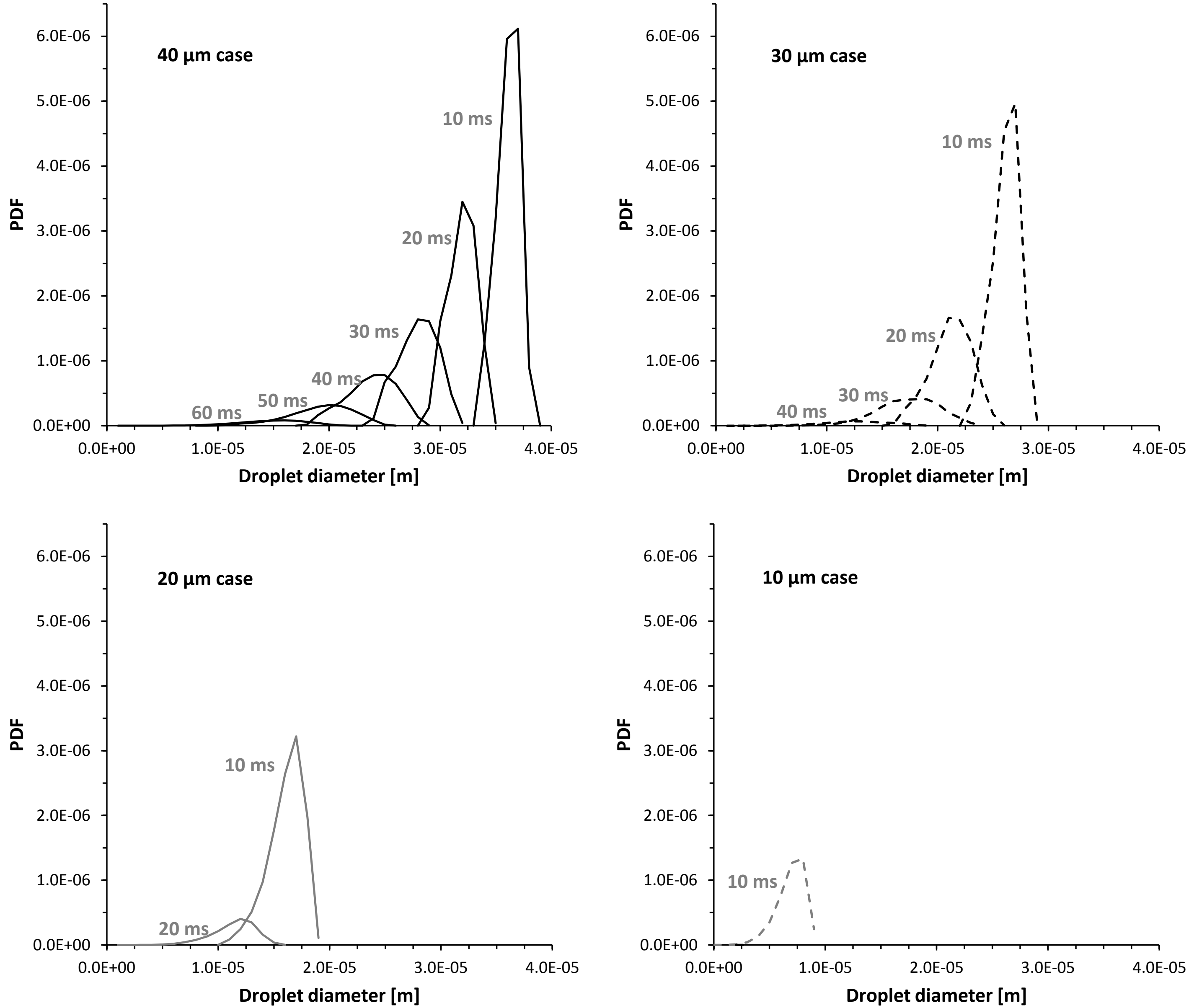
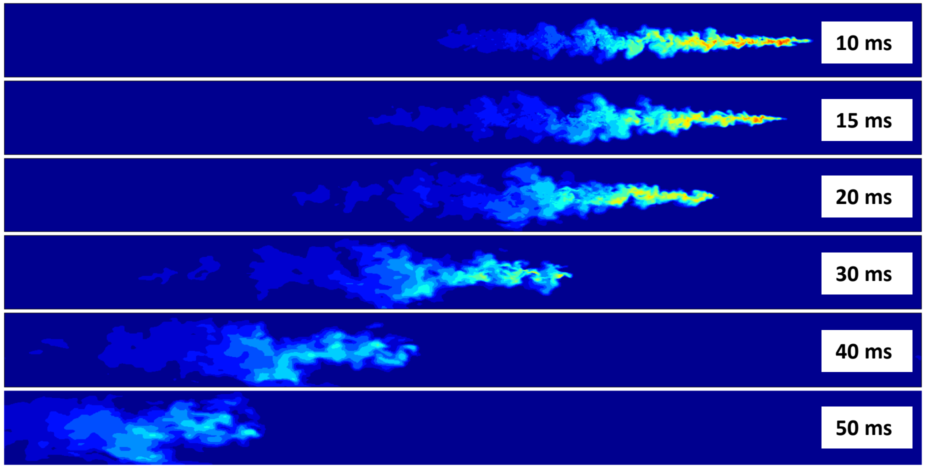
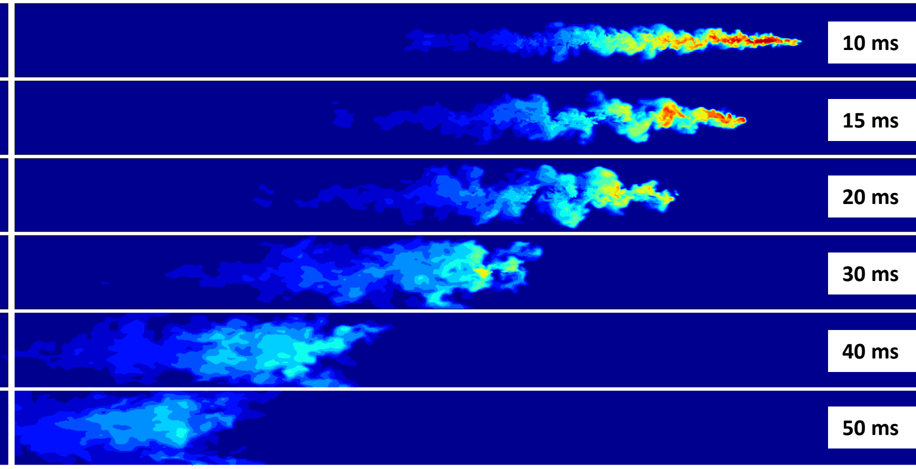
SCR spray droplet sizes



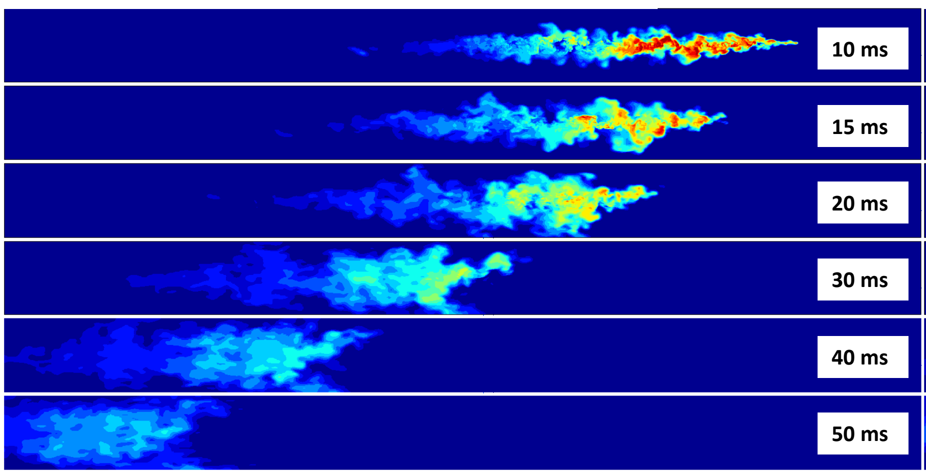
SCR vapor evolution



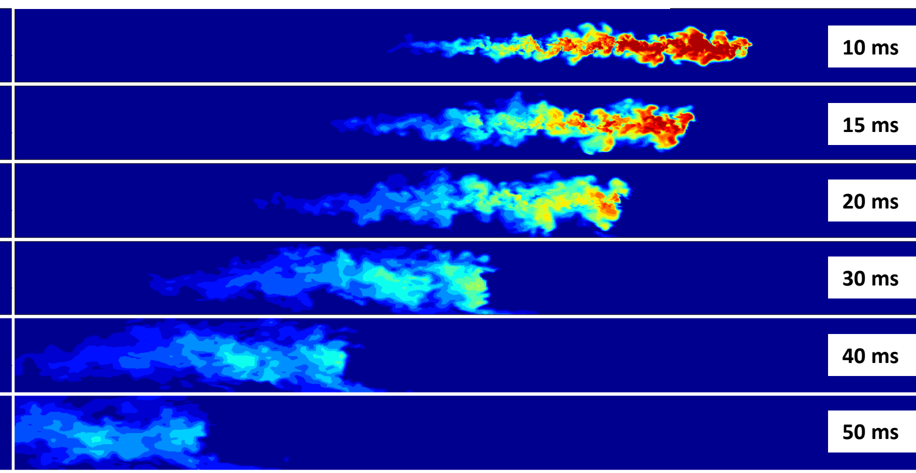
40 µm droplets



30 µm droplets



20 µm droplets



10 µm droplets

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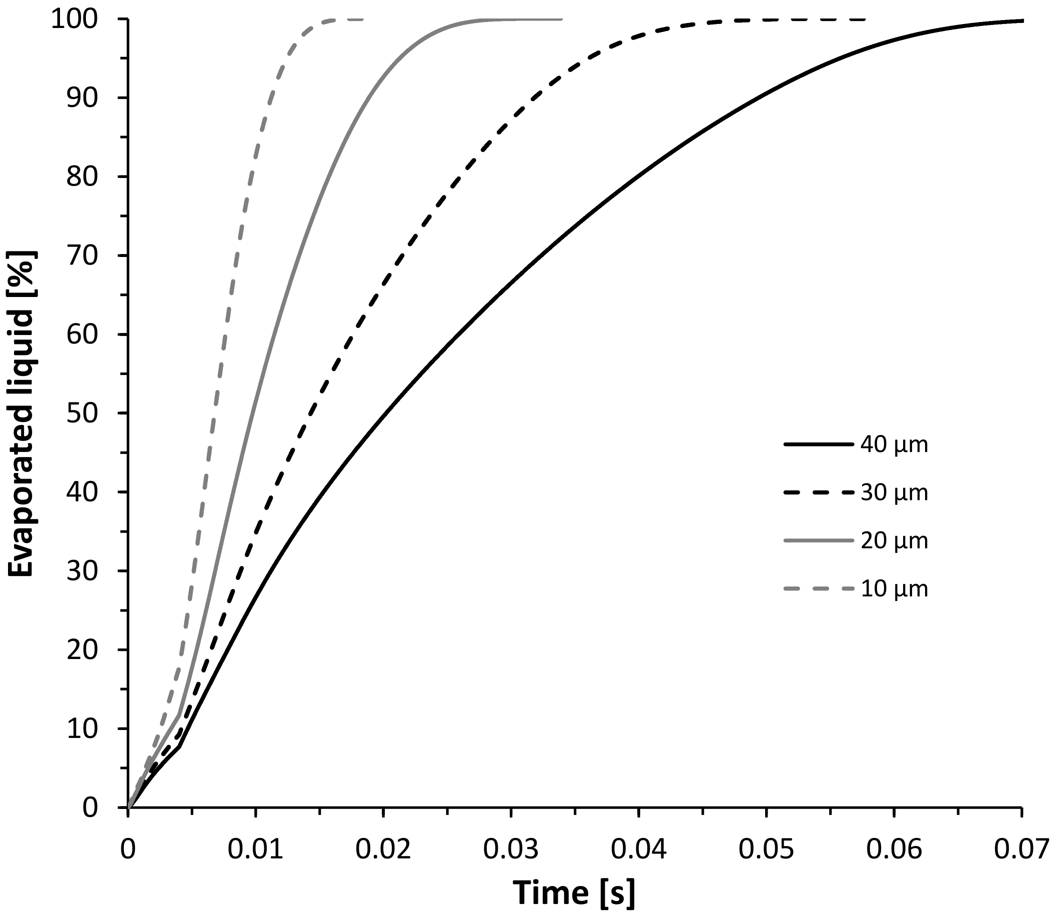
The scale is from 0 (blue) to 8% (red) vapor concentration.

SCR spray evaporation



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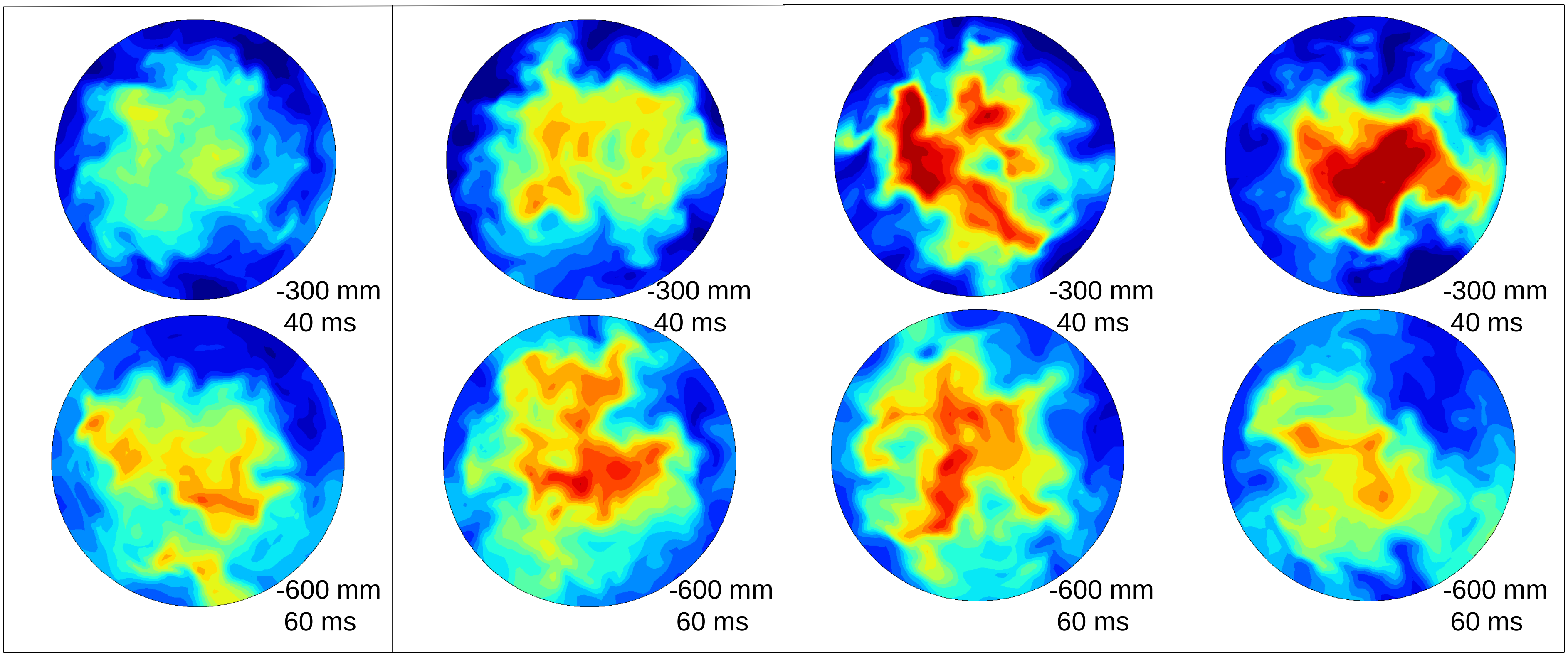
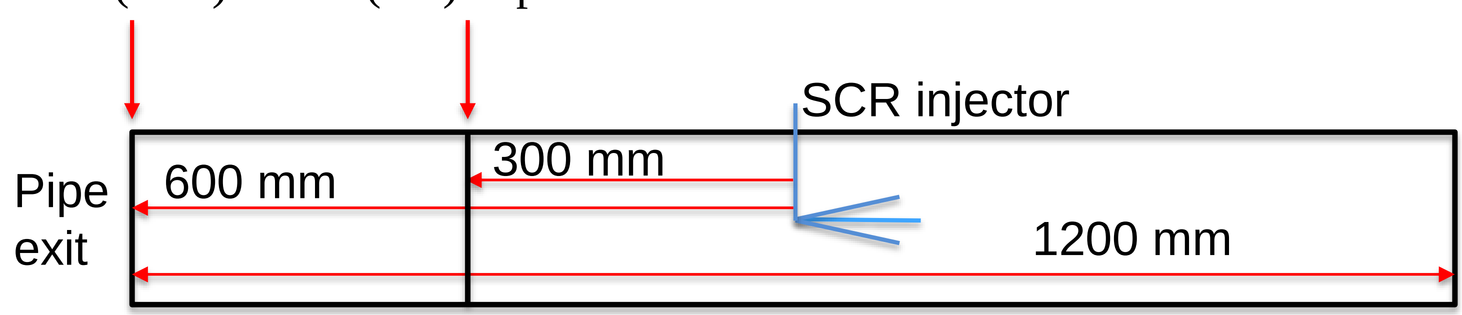
SCR vapor distribution



40 µm 30 µm 20 µm 10 µm

The scale is from 0 (blue) to 3% (red) vapor concentration.



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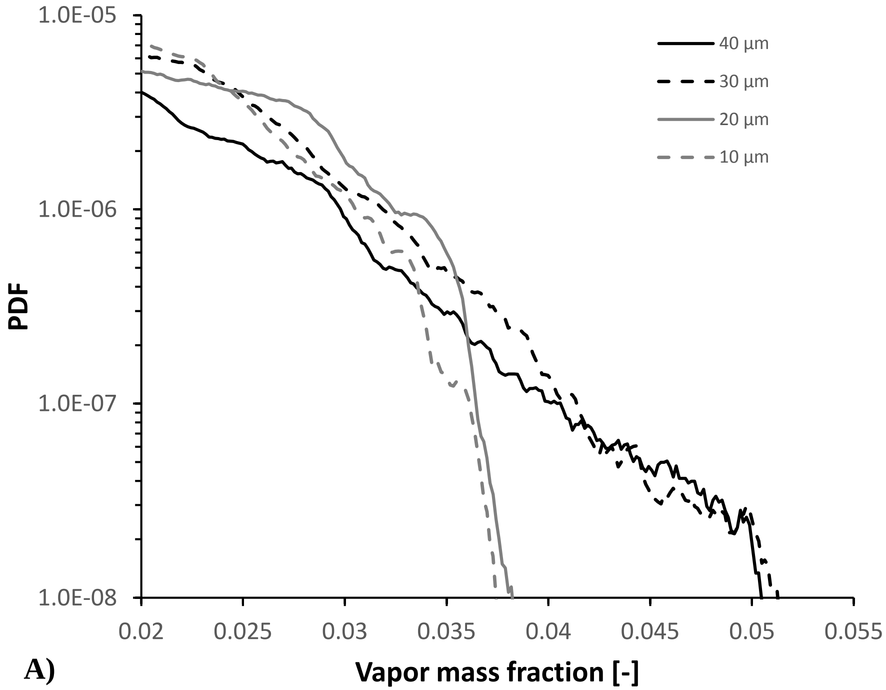
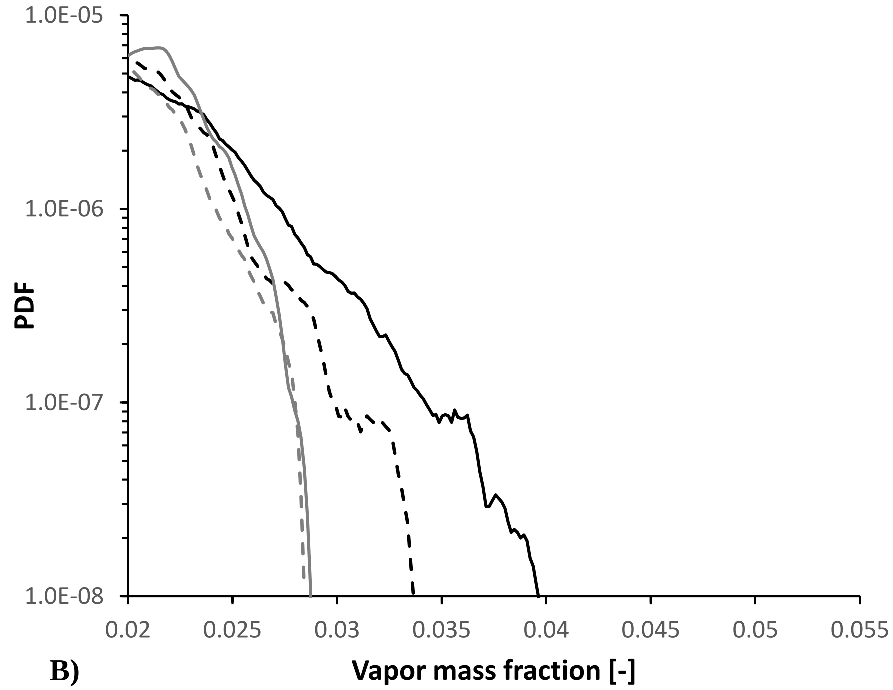
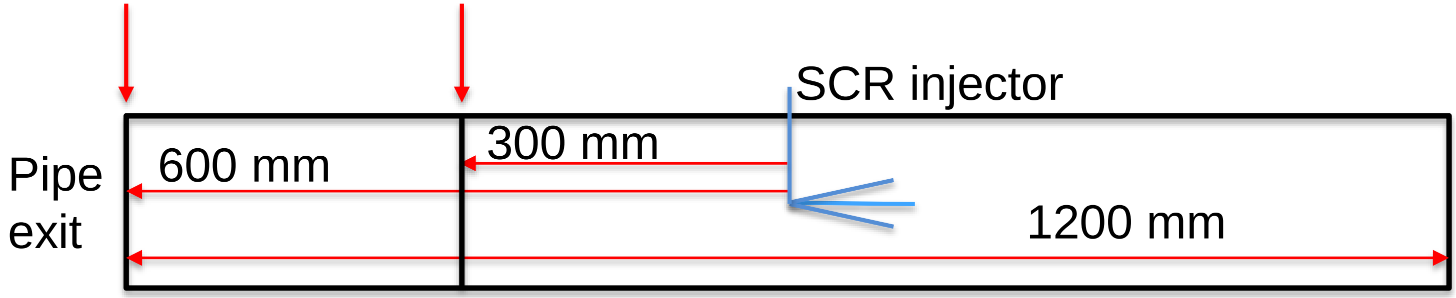
SCR vapor distribution





40 ms

60 ms



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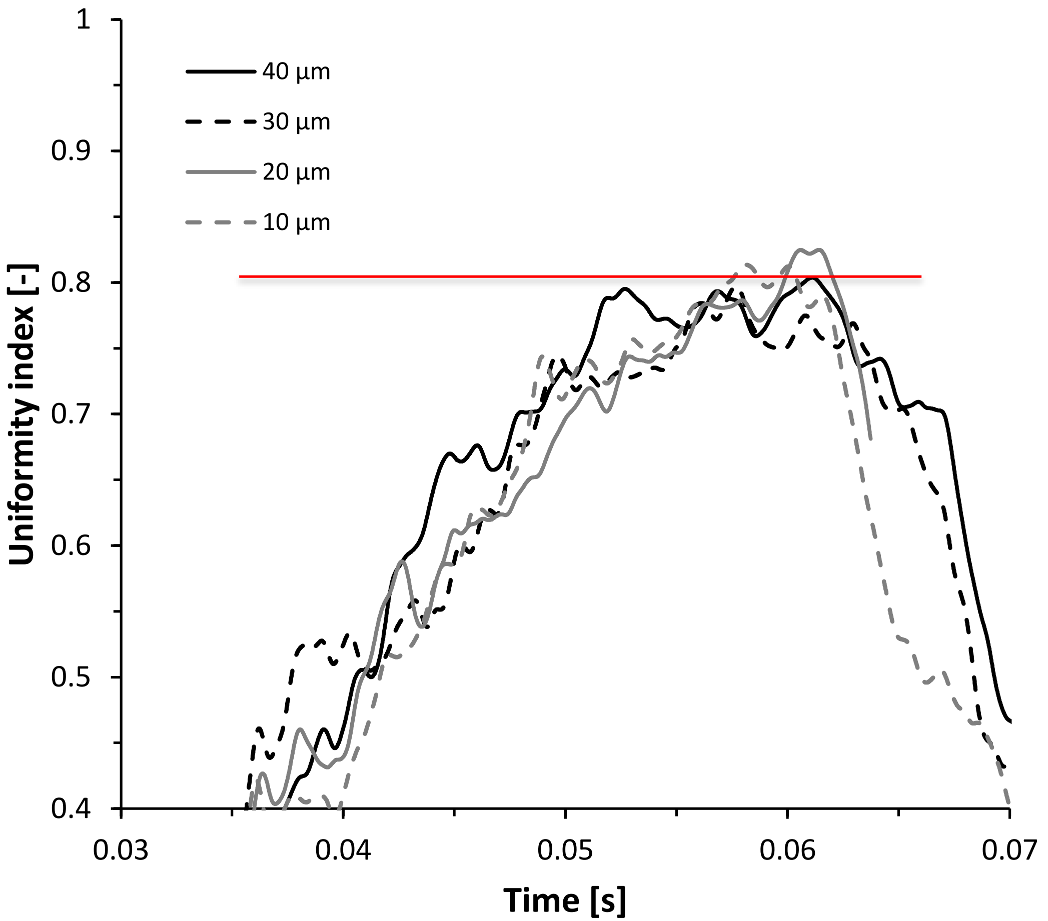
SCR vapor uniformity

$$UI = 1 - \frac{\sum_i^N |Y_i - \bar{Y}| A_i}{2|\bar{Y}| \sum_i^N A_i}$$



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Situation at the end of the pipe

Conclusions

- Accurate turbulence modeling (LES) was applied for the 1st time in an SCR system simulation
- High Reynolds number turbulent pipe flow was in good agreement with experimental data
- The droplet evaporation rates were strongly correlated with their size. On the other hand, vapor distribution at the pipe exit was not.
- The strong vapor mixing observed in a short distance upstream the pipe exit suggests that more uniform vapor distribution could be achieved by a relatively modest pipe lenght increase.

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