Validation of Computational Fluid Dynamic Simulations with Background Oriented Schlieren Technique

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Introduction

A critically assessed and experimentally validated numerical AP ion source model opens a gateway to a whole new design approach, i.e., from trial and error towards model driven engineering. Within such models, fluid dynamics plays a major role due to several substantial gas flows present in an API source.

The validity and applicability of any CFD model along with the required specific model assumptions generally need to be verified experimentally.

Previous research:

- A digital model of an atmospheric pressure ion source was generated using Computational Fluid Dynamics (CFD) in collaboration with the RWTH Aachen (University of Aachen, Germany). This model was further validated using Particle Image Velocimetry (PIV) [3].
- Since PIV as validation method is experimentally and also cost-wise rather demanding, the community is seeking for alternatives. Last year, we presented the principle application of the Background Oriented Schlieren Method (BOS)[7] to visualize the hot gas flow in an Bruker Multi Purpouse Ion Source (MPIS) [2].

Our approach:

- The advantages of the Background Oriented Schlieren method as a supporting tool for validation purposes are demonstrated. The BOS apparatus used shows the refractive index gradient caused by the temperature differences between heated gas flows and the cold background gas.
- The results of fluid dynamic calculations are not directly comparable with Schlieren images. Howerver, from these datas synthetic Schlieren images can be calculated. [6]

Summary:

- Although BOS generates much less data as PIV, it is nevertheless capable to determine gross deviations from model and experiment.
- Images with short exposure times show even the turbulent flow in atmospheric pressure ion sources.

Methods

Ion Source:

- Multiple Purpose Ion Source (MPIS)

BOS:

- Camera: Canon EOS M
- Objective: EF-M 18-55mm f/3,5-5,6 IS STM
- Aperture: 29, - ISO: 400
- Pattern: 8x10e8 Dots/m^2, Dot size 0.3 mm

CFD:

- COMSOL Multiphysics© (V 4.4) COMSOL, Inc.
- ANSYS© CFX-12.0 Solver. ANSYS, Inc.

Calculation & Plotting:

- Python 2.7.5, http://www.python.org
- NumPy 1.7.1, http://www.numpy.org
- Matplotlib 1.2.1, http://www.matplotlib.org
- scipy 0.12.0, http://www.scipy.org
- OpenPIV 1.0.7, http://www.openpiv.net

From CFD to Synthetic Schlieren Images

CFD-Simulation:

For prove of concept a simplified, rotationally symmetric model of the nebulizer was used.

Boundary conditions:

T_Neb = 553 K
v_Neb = 3D parabolic, v_max= 2.8 m/s
p_out = 1 atm

Fluid properties:

standard air
a) laminar
b) turbulent (k-ε-model with IT = 0.002, LT = 0.001 cm)

Output: irregular mesh of fluid density

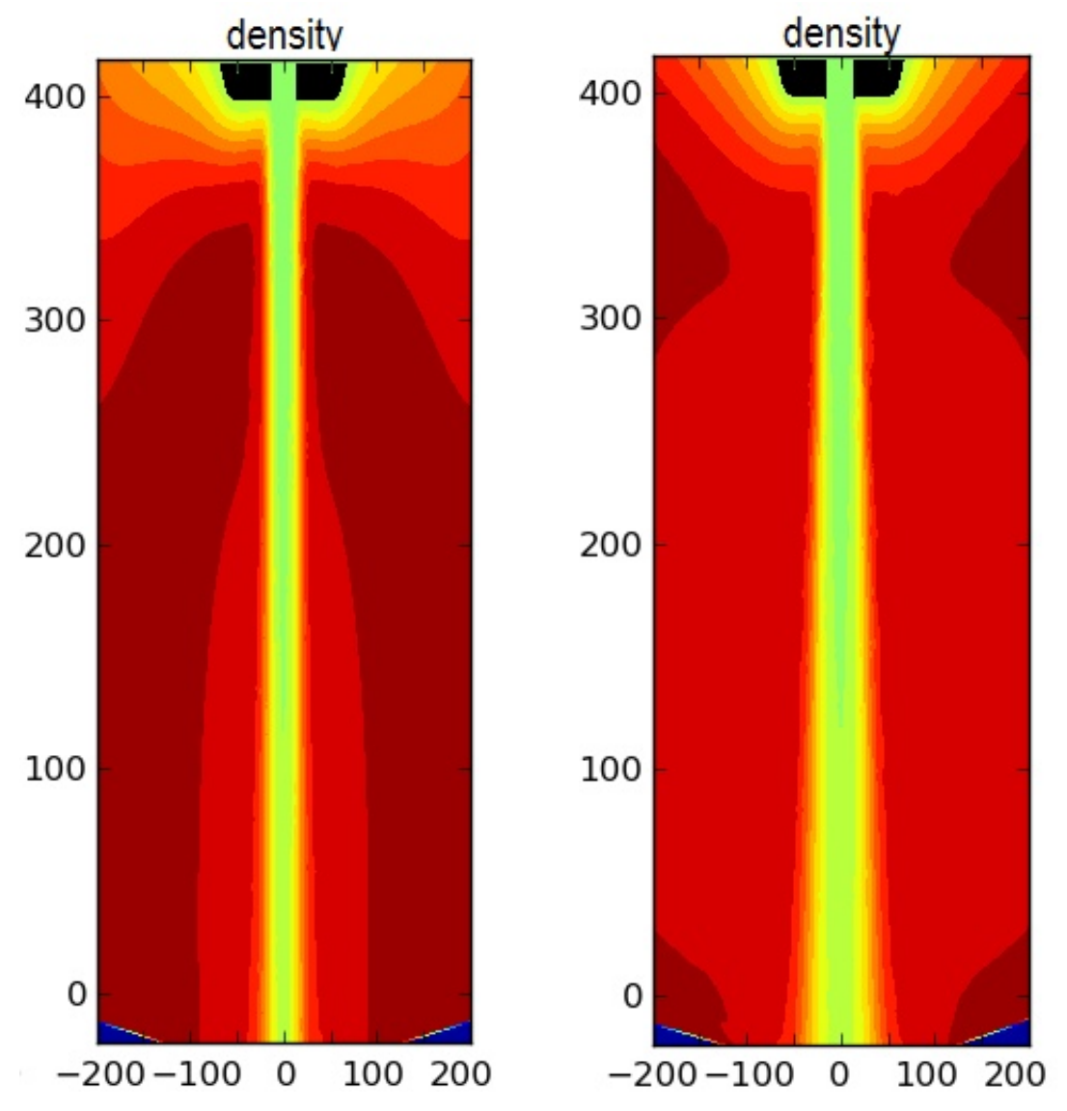


Fig. 1: Interpolated density field from the laminar (left) and turbulent (right) simulation conditions

Interpolation:

Delaunay triangulation over the irregular mesh

Output: regular 3D-array of fluid density (Fig. 1)

Calculation of the refractive index:

Refractive index n in each element of the array from the density ρ as determined with the Gladstone-Dale equation:

$$n = \rho \cdot G + 1$$

with G = 0.23e-3 m^3/kg (Gladstone-Dale constant [4])

Output: regular 3D-array of the refractive index distribution

Light deflection:

As light travels through a continuous medium with a spatial gradient of refractive index, it is deflected. If the gradient is small, the deflection angle is given by the integration along the line-of-sight (projection along z-axis):

$$\epsilon^x = \int_0^L \frac{1}{n(x,y,z)} \cdot \frac{\partial n(x,y,z)}{\partial x} \mathrm{d}z$$

For the numerical calculation of the deflection angle (in a 3D-array with elements n(i,j,k), where k indicates axis of projection) a discretization (dz->Δz) of the integral is used:

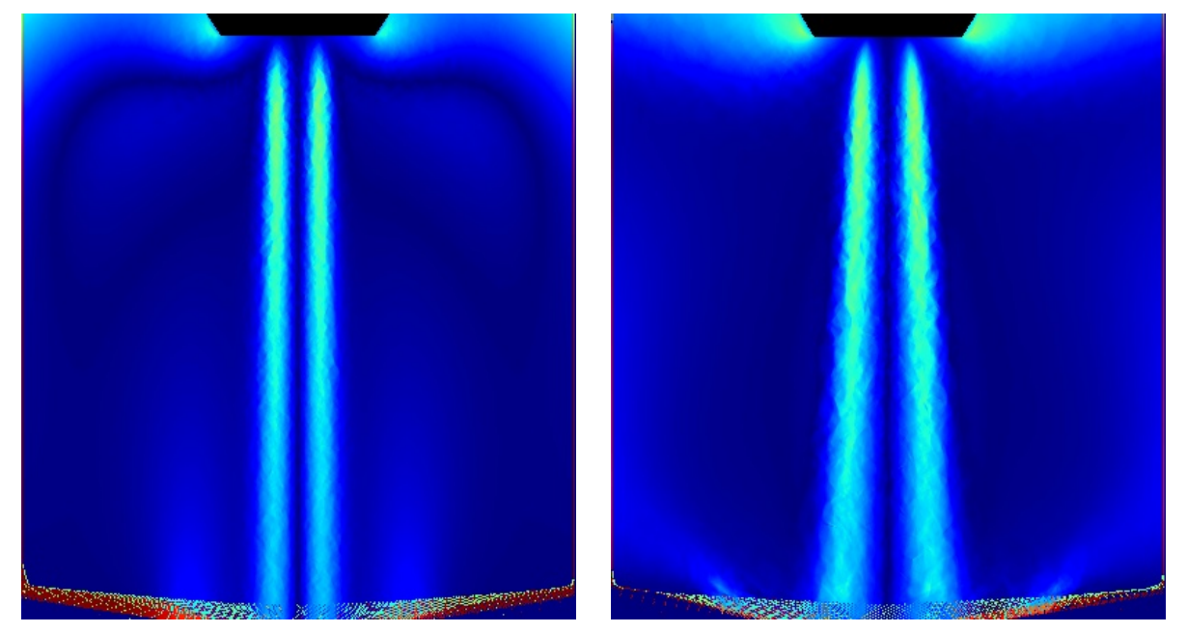
$$\epsilon^x_{i,j} = \sum_k \frac{1}{n(i,j,k)} \cdot \frac{\Delta n(i.j.k)}{\Delta x} \Delta z$$

$$\Delta n(i,j,k) = n[(i+1,j,k)$$

$$\Delta x = \Delta z = 1$$

Validation:

Contrasting juxtaposition of the simulated Schlieren image and the experementally measured Background Oriented Schlieren (BOS) pictures (Fig.: 2)



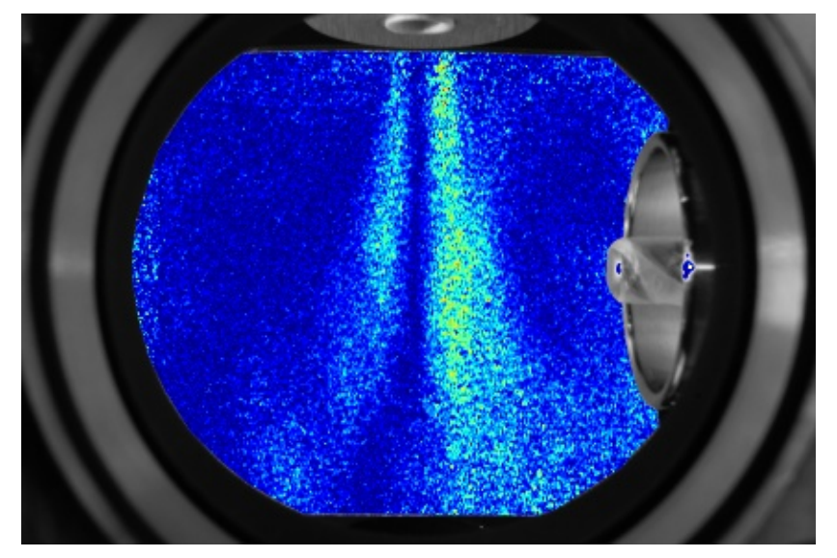


Fig. 2: Synthetic (simulated) Schlieren images for laminar (top left) and turbulent (top right) fluid flow. The picture at the bottom right corner shows the experimentally measured BOS image

Outline

CFD-Simulation

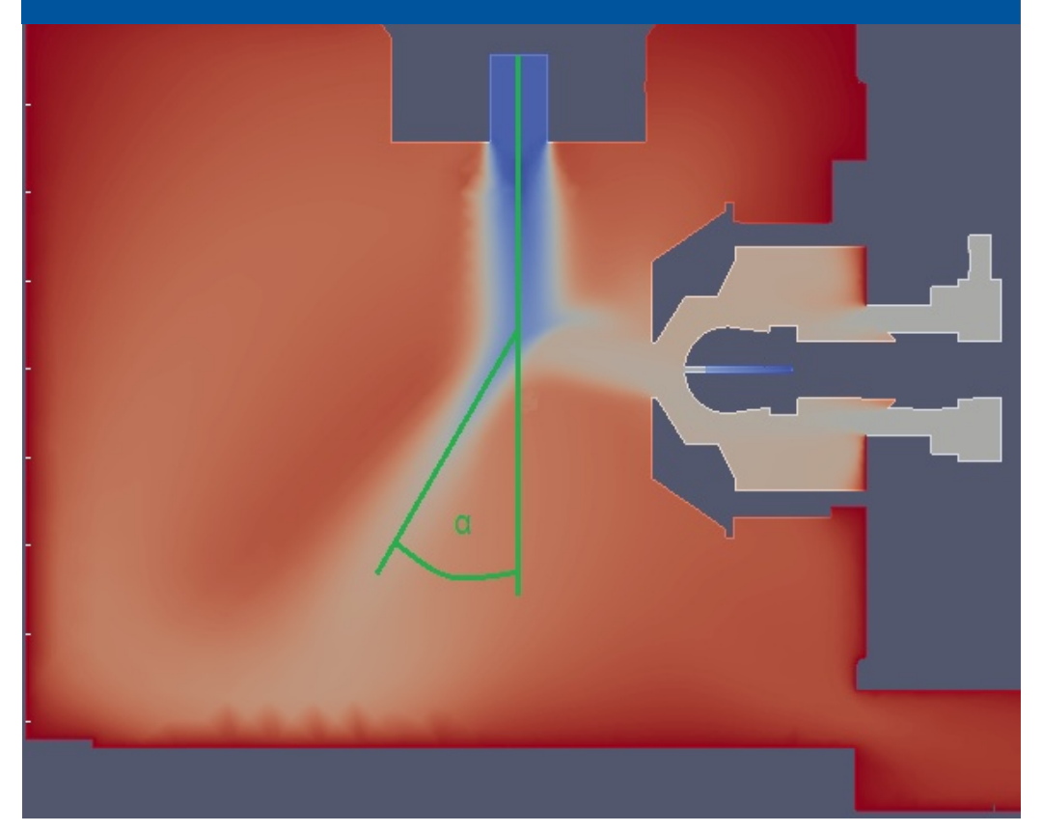


Fig. 3: Interpolated density field from the CFD simulation of the MPIS [3]. Nebulizer pressure: 1.8 bar (1.1 L/min fluid flow); gas temperatur 183 °C; drygas flow: 1.6 L/min at a gas temperature of 131 °C

Neb. Flow

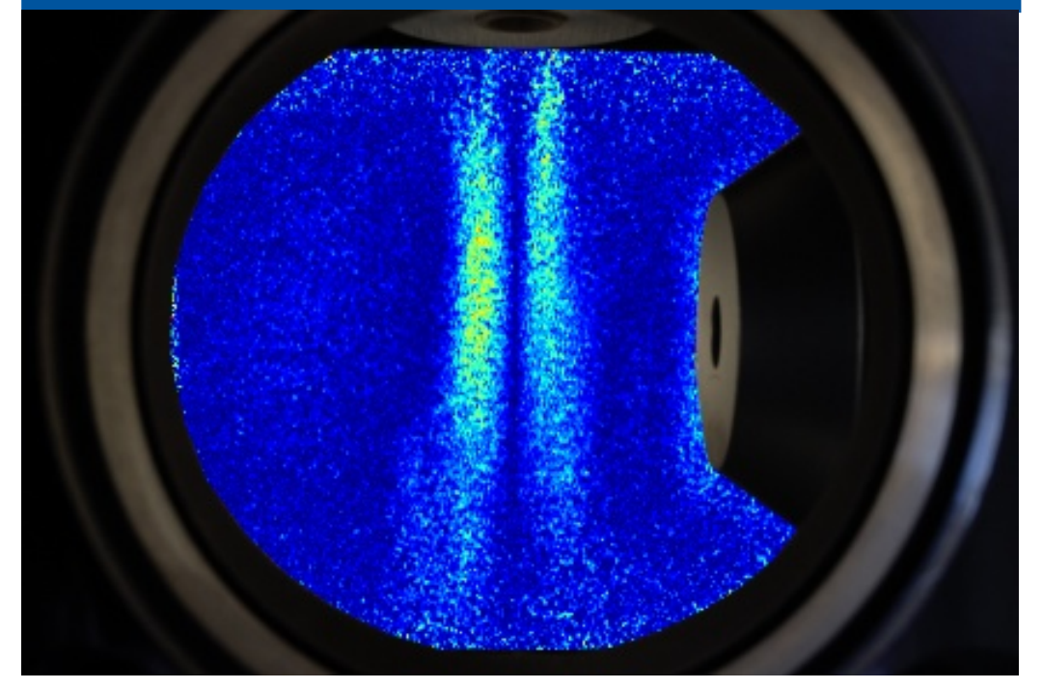


Fig. 4: Undisturbed Nebulizer gas flow. The gas temperature was set to 206 °C (measured 183 °C); fluid flow: 1.8 bar corresponding to 1.1 L/min

Drygas Flow

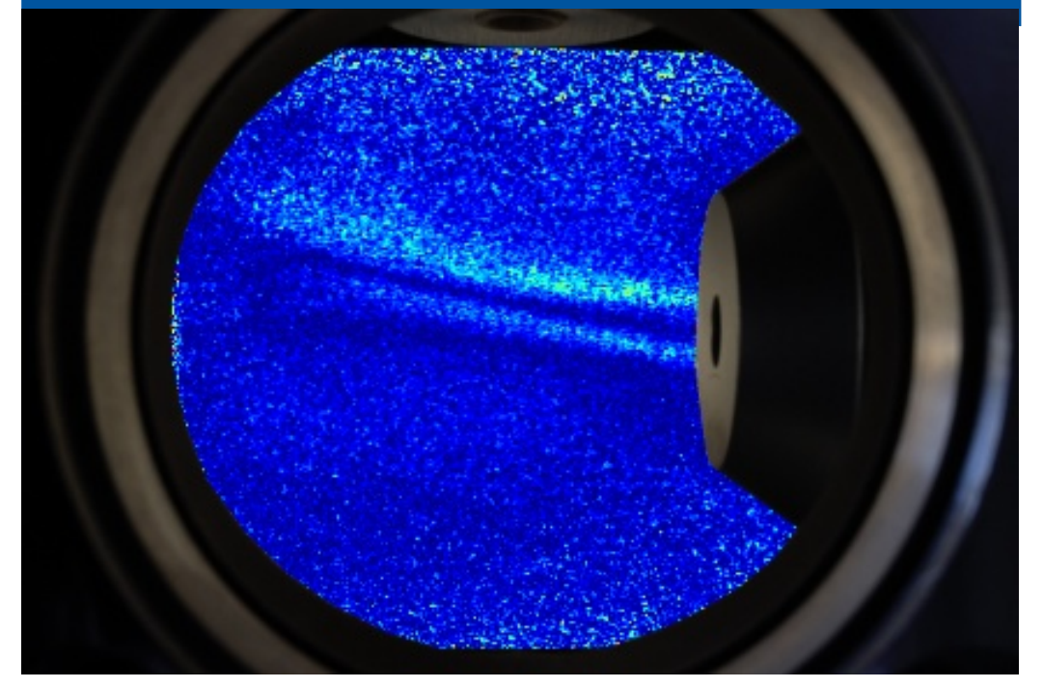
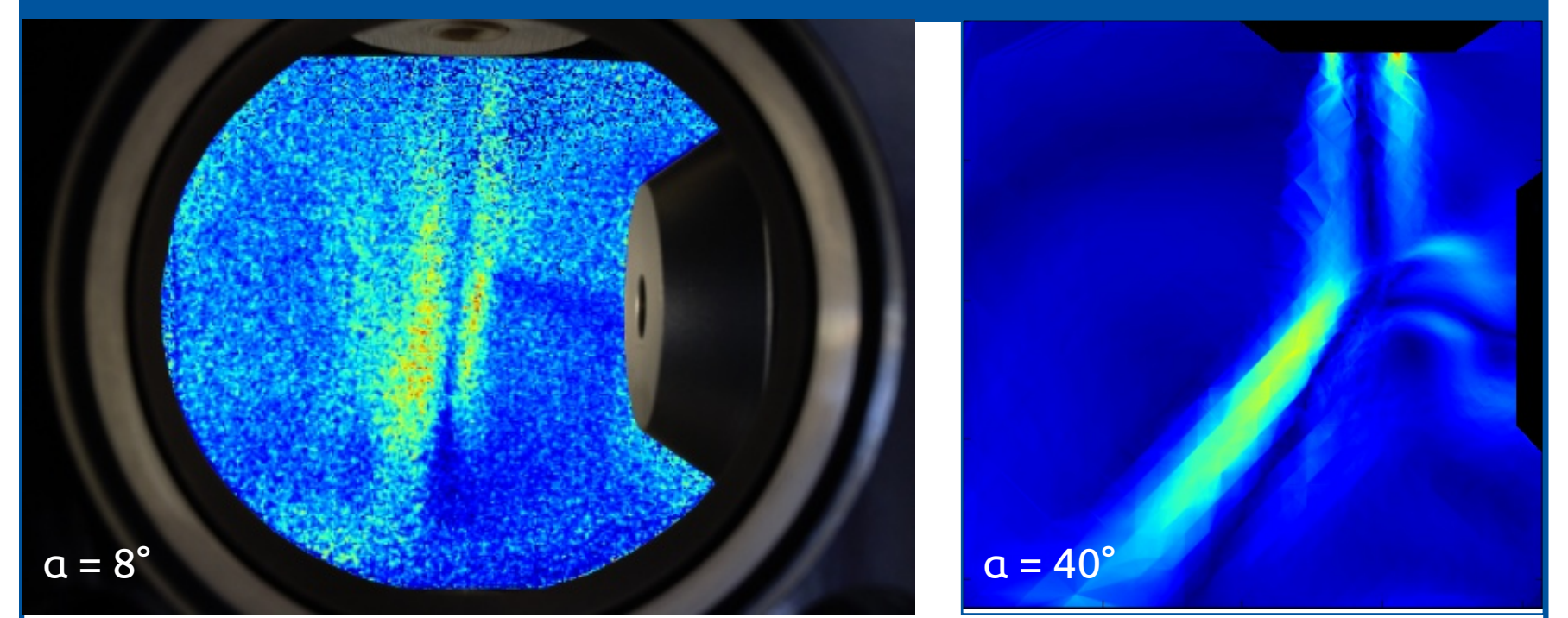


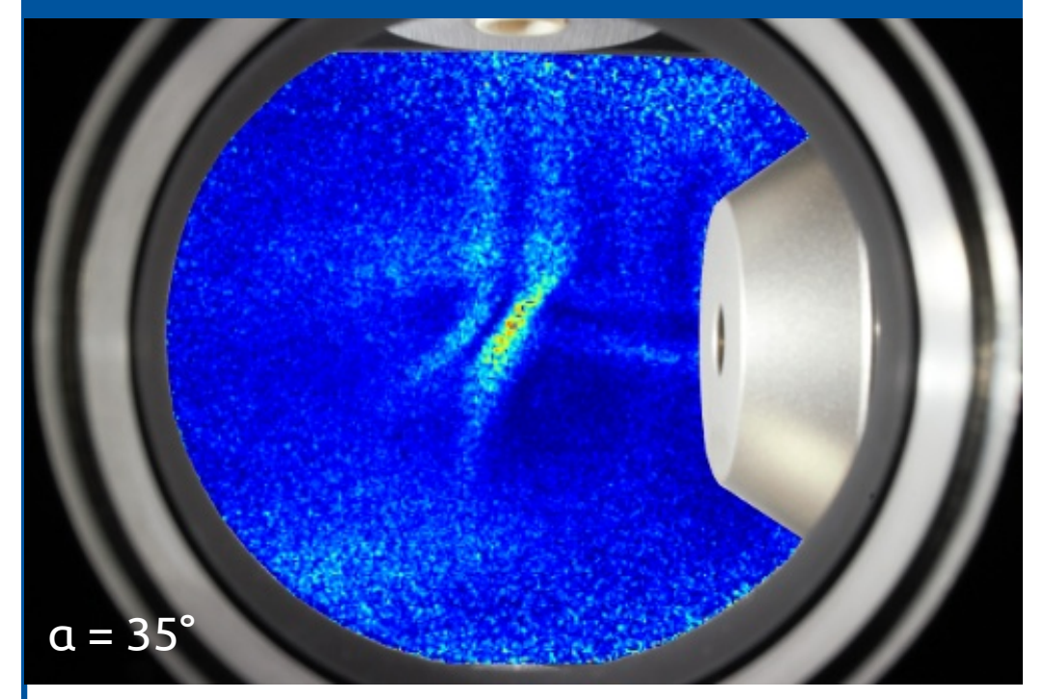
Fig. 5: Undisturbed drygas flow. The temperature was set to 350 °C (measured 120 °C); fluid flow: 2.5 L/min, the net flow is 1.6 L/min , the capillary sucks approximately 0.85 L/min

Experiment vs. Simulation

1.6 L/min

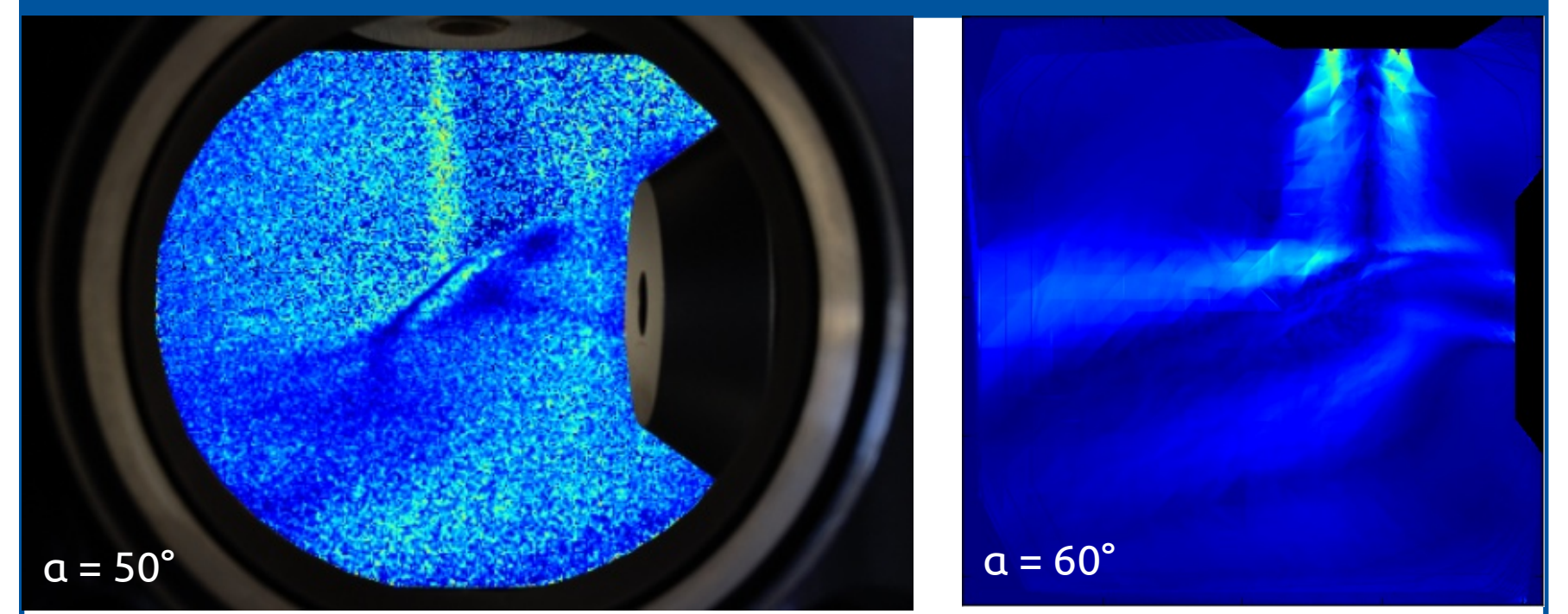


2.0 L/min



- Interaction of both gas flows inside MPIS
- BOS and synthetic Schlieren images with constant Nebulizer pressure
- The CFD model was already validated with PIV [3]

2.5 L/min



3.0 L/min

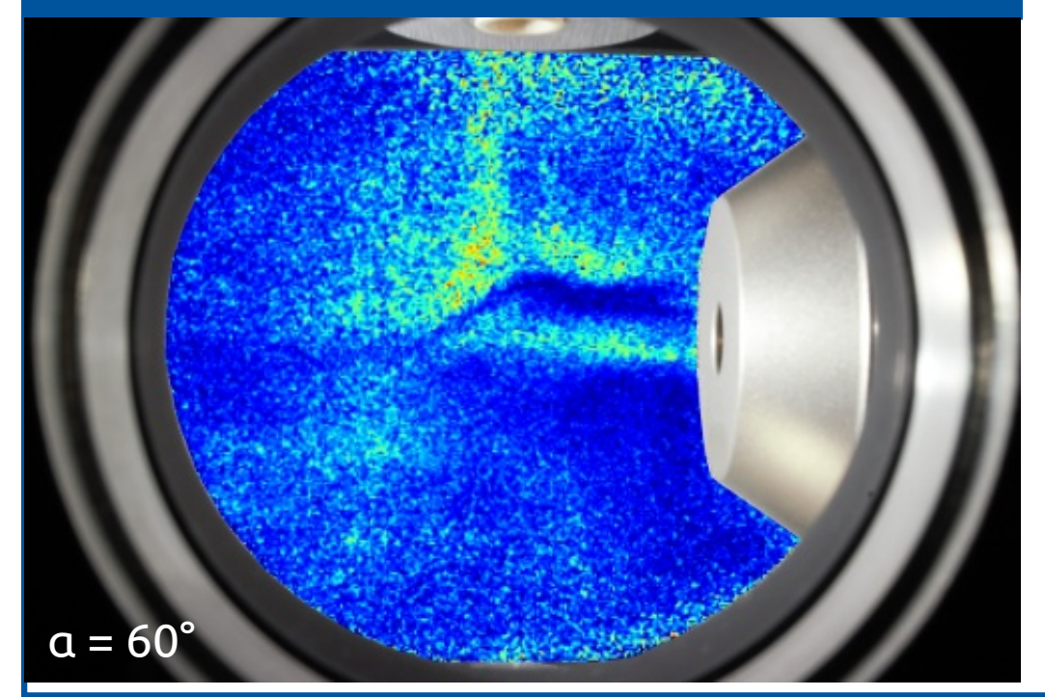


Fig. 6: Measured and simulated Schlieren Images at different drygas flows, nebulizer pressure at 1.8 bar. The deflection of the Nebulizer flow by the drygas is clearly visible. left row: experiment; right row: synthetic Schlieren images

Short Time Exposure

- Generally, simulations and measurements show only averaged density fields. The exposure time is about half a second. With the help of a flash light, exposure times down to miliseconds are achiveble.
- The turbulent structure of the interacting gas flows becomes clearly visible in the "snapshots".
- The complex structures (e.g. vortices) are not stable. Within short periods, the pattern change rapidly and dramatically
- These highly visible transient patterns are not visible in the BOS-pictures with longer exposure times.

"Low Flow" Conditions

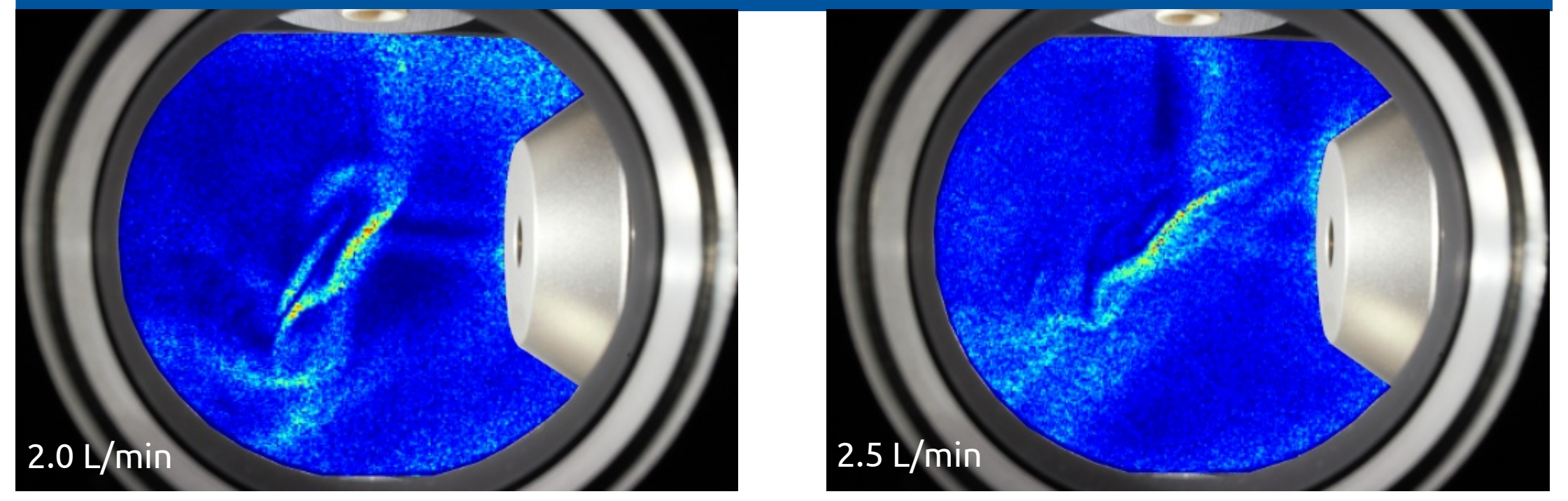


Fig. 8: Not averaged stream interactions for two diffrent drygas flows at 131 °C. Nebulizer pressure was constantly at 1.8 bar and a temperature of 183 °C

"High Flow" Conditions

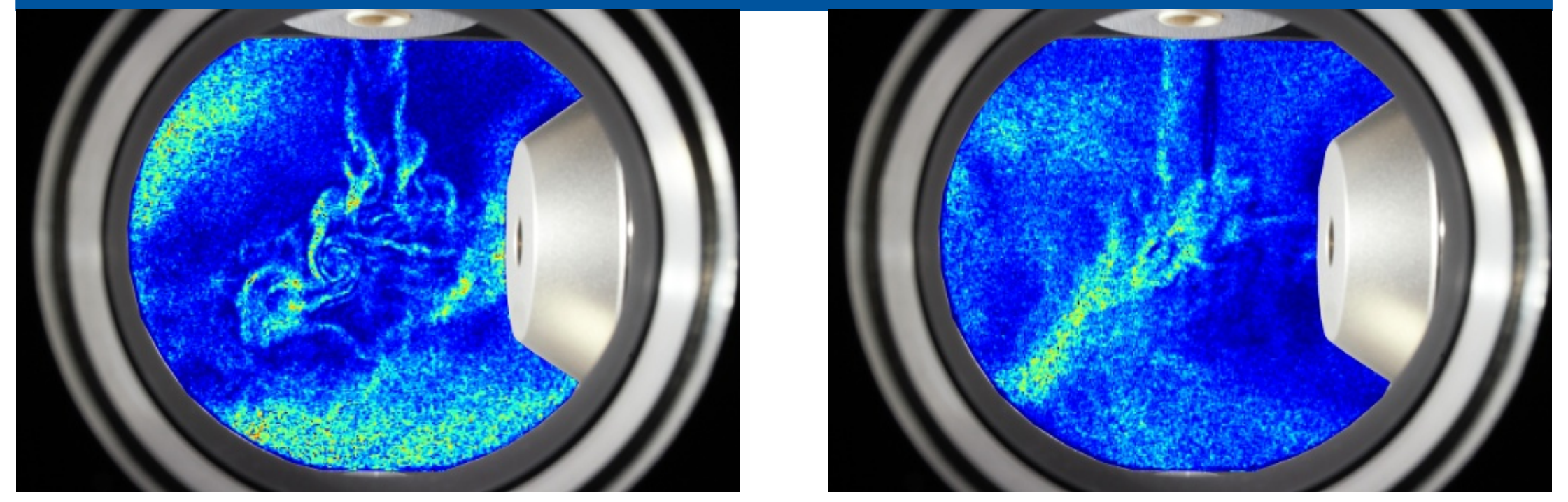


Fig. 9: Not averaged stream interactions, with 3.8 L/min drygas flow at 131°C and a Nebulizer pressure of 5.7 bar at 183 °C. Both images are taken with a time diffenrence of less than 30 seconds

Deflection Angle

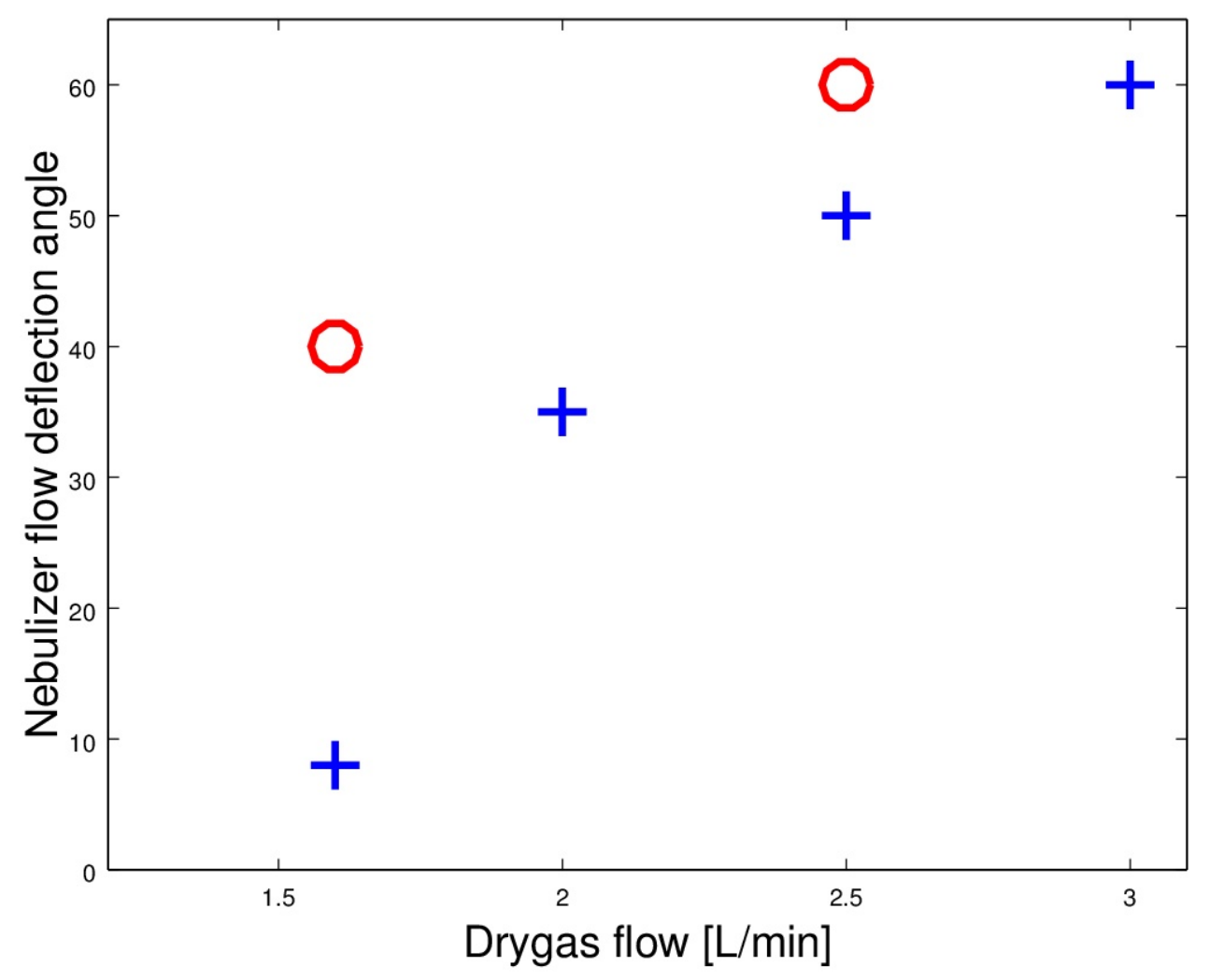


Fig. 7: Dependence of the deflection angle α form the drygas flow. The data form the simulations are shown as red circles, the BOS-pictures with blue crosses.

- There in an offset between synthetic Schlieren images and BOS data of approximitly 0.5 L/min.
- There are inaccuracies in the determination of the capillary flow. The mass flow is determined by the temperature of the capillary, which in turn depends on drygas temperature and flow.

Results & Discussion

Synthetic Schlieren images

- Schlieren images were successfully generated from the results of fluid-dynamic calculations, either from a simplified model or at true experimental conditions.
- In all probability in all CFD simulations the application of a turbulence model is necessary.
- The long time exposure gives only an averaged picture. In reality turbulences and oscillations strongly affect the fluid flow. These turbulence are not visible in the simulated Schlieren images since an equilibrium state is calculated from the CFD-solver.

Experiment vs. Simulation

- The dependence of the nebulizer deflection angle from the drygas flow is obvious in both the BOS and in the synthetic Schlieren images.
- The deflection angles of the simulated/synthetic Schlieren images do not match. The calculated angles are larger than experimental values for the same drygas flow. However both data sets converge at higher drygas flows.

Known issues

- The actual Drygas flow is coupled to the capillary gas flow (0.8 L/min in the experiment) into the mass spectrometer. Since this interaction is not treated properly in the simulation the actual drygas flow between the simulation and the experiment may differ.
- Since the capillary inlet is located behind a sprayshield the actual capillary gas flow could not be observed using PIV for validation.
- In the setup used the drygas heats the glas capillary indirectly. Therefore the drygas temperature affects the capillary gas flow, thus varies with different drygas temperatures.
- Because of experimental limitations, the validation by PIV was only performed at room temperature. Standart atmospheric pressure ion source operate at temperatures 100 to 200 degrees above RT. This renders the a the validation of the CFD model.

Conclusions

- typical steady state CFD simulations severely underestimate the highly dynamic processes in atmopheric pressure ion sources.
- The combination of simulated Schlieren images and the BOS method is demonstrated to be a great tool for the validation of CFD simulations and the dependences on various physical parameters.
- The great advantage of this setup is the straigth foreward implementation and simple operation of the experiments.

Outlook

- An improved experimental setup and workflow may give new insights into the highly dynamic processes in atmospheric pressure ion sources.
- Moving pictures are the next step for a better understanding of the processes taking place inside the ion source.
- It is envisioned to visualize the interaction of the flows from a different angle. A simulation of such Schlieren images is straigth forward, the experimental setup however is much more difficult. With a comparison from two (perpendicular) angles, a validation could be even more accurate.

Literature

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