Visualization and optimization of the fluid dynamics in high-flow atmospheric pressure ion sources, using the Background Oriented Schlieren method (BOS)

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Introduction

- In common API sources several high-volume gas flows interact, particularly in hyphenation with LC
- Without further measures, the resulting complex fluid dynamics leads to increased ion and neutral dwell times resulting in peak broadening effects [1]
- The investigation of this complex fluid dynamics, e.g. with particle image velocimetry (PIV) techniques, leads to considerable experimental effort [2]
- Computational fluid dynamic (CFD) models need to be validated experi-mentally

- A Bruker Multi Purpose Ion Source (MPIS) was equipped with a custom gas exhaust system
- This system called Active Elevated Floor (AEF) allows automated con-trol of an additional sheath gas flow supplied to the source

- The Background Oriented Schlieren (BOS) technique builds on the distortion of imaging of deliberate „backgrounds" by the light de-flection of density gradients [3]
- BOS allows determining tempe-rature / density gradients of gases without sophisticated optical equipment

Methods

Chromatography:

Analyt: Pyrene in Me/Water (9:1), 20 µL / 100 nmol/L
LC: Me/Water (9:1), 1 ml/min
T_Neb.: 425°C
Drygas: 300°C, purified Air
MS: Bruker MicrOTof

BOS:

Camera: Canon EOS 600D
Objective: 18 – 50 mm, deactivated AF
Pattern: 8 * 10⁸ Dots/m², Dot size 0.3 mm
Aperture: 32
Exp.Time: 1/3 s

Cross Correlation:

PIV: OpenPIV [4]

AP Ion Sources

Multi Purpose Ion Source (MPIS)

The standard MPIS is used for various chromatographic coupling methods, both LC and GC are possible. Numerous AP ionization methods may be used, e.g., APLI, APCI, ESI, and APPI.
Due to the original location of the drain and the highly variable gas flows the analyte path is more or less undirected and essentially uncontrolled.

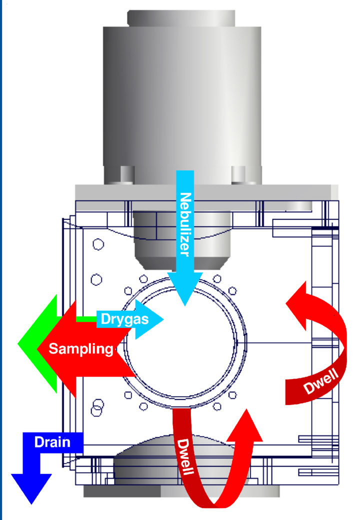


Fig. 1: Standard MPIS in LC-APLI con-figuration

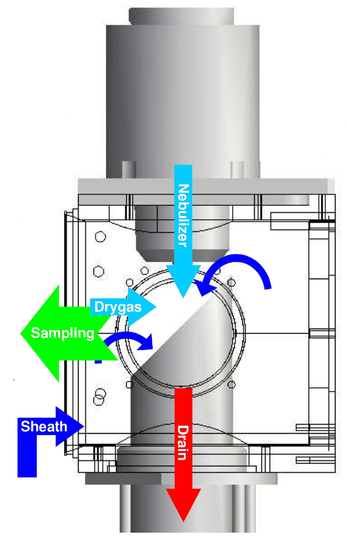


Fig. 2: Custom made modi-fication of the MPIS with the *AEF*

Active Elevated Floor (AEF)

The modifications to the ion source enclosure represent only minor changes of the basic layout, both implementations are largely comparable.
The utilization of the AEF unit enables the automated control of the gas transport in this particular source design.
The drain is located across from the nebulizer, the sheath gas flow through the original drain opening is regulated by a mass flow controller.

Principle of the BOS-Method

1.) Experimental Setup

The experimental setup, compared to the classical Schlieren technique, is much less elaborate. The system is built without expensive and difficult to adjust optical equipment. In front of a random, computer generated pattern (background), an object is placed, which changes the optical density of the environment, e.g., a candle, lighter, or hair blower.

With a standard SLR two pictures are taken, one with and one without the change of the optical density. Both, the pattern and the object, need to be located in the same depth of field.

The refractive index gradient causes light deflection and leads to two slightly differing pictures. The effect is the same that causes a fata morgana.

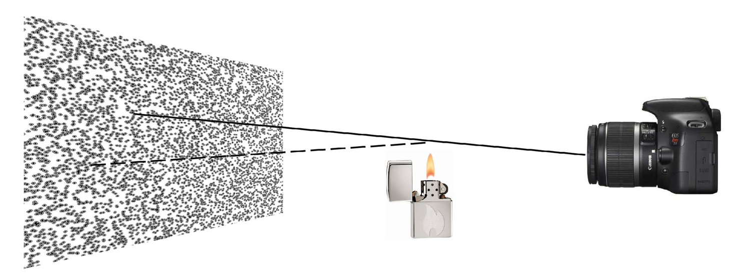


Fig. 3: The background is decorated with the random pattern. Light beams are deflected under different angels by the hot air above the flame due to the refractive index gradient. The differences are imperceptible to the naked eye

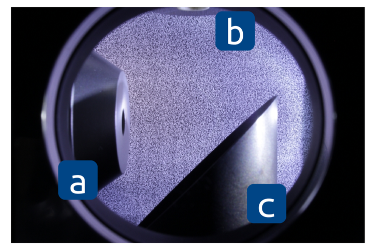


Fig. 4: The picture shows the pattern, installed in the ion source.
The camera looks rectangular to the dry gas and the nebulizer gas flow.
The pattern is illuminated with a powerful LED flashlight through a glass window at the front of the ion source.
a) spray shield, b) nebulizer, c) AEF

2.) Taking the Pictures

The experiment consists of a sequence of two steps. First, the background is photographed without distorted optical density. In the second step, the refractive element, in this case, the gas streams are brought into the field of view of the camera and a second photo is taken.

The dot density and dot size of the random background pattern used, depends on the resolution of the camera employed. Each dot of the pattern should be mapped to at least three pixels of the CCD of the SLR.

If the pattern and the refractive element are in the same depth of field both will be sharply mapped. To achieve this, a large aperture is used leading to long exposure times or requires a high amount of illumination. Between taking both pictures, the setup must not be moved.

The camera records pictures in raw format, then they are converted to bitmaps, and the color information is removed. The batch processing of pictures is performed with the "Image Magick" software collection.

3.) Cross Correlation

By the implementation of the BOS method the main effort of Schlieren detection is transferred to the computer, which performs the actual work of precise image correlation.

The software uses was originally programmed for PIV (particle image velocimetry) analysis; the algorithm for the 2D cross-correlation are basically the same.

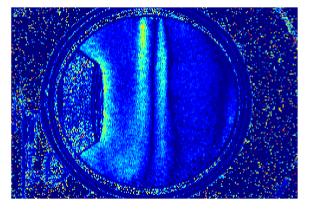


Fig. 5: Horizontal deflection of the light beams. No dry gas used. The nebulizer is operated with a pressure of 3 bar and a temperature of 425°C. The air in close vicinity to the spray shield was heated by the hot surface. Areas without defined pattern (e.g. MPIS housing) lead to random signals.

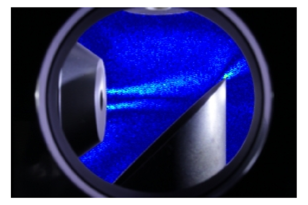


Fig. 6: The vertically light deflection is clearly discernible The MPIS is equipped with the AEF device. Dry gas flow 4 L/min; temperature 300 °C. The interaction of the gas flow with the AEF is clearly visible.

4.) Processing & Interpretation

The computer analysis results in two 2D arrays containing the displacement vectors of the pattern in vertical and horizontal direction. The plots correspond to Schlieren images taken with a horizontal and vertical knife edge.

The interpretation of the plots requires a basic understanding of fluid dynamical properties of the source, however the method is a nice tool for the evaluation of CFD models.

Schlieren Pictures

The images visualize the flow pattern resulting from two different dry gas flows and two different nebulizer pressures, respectively.

Each box shows two images: the upper picture visualizes the vertical, the lower the horizontal light deflection/density gradient.

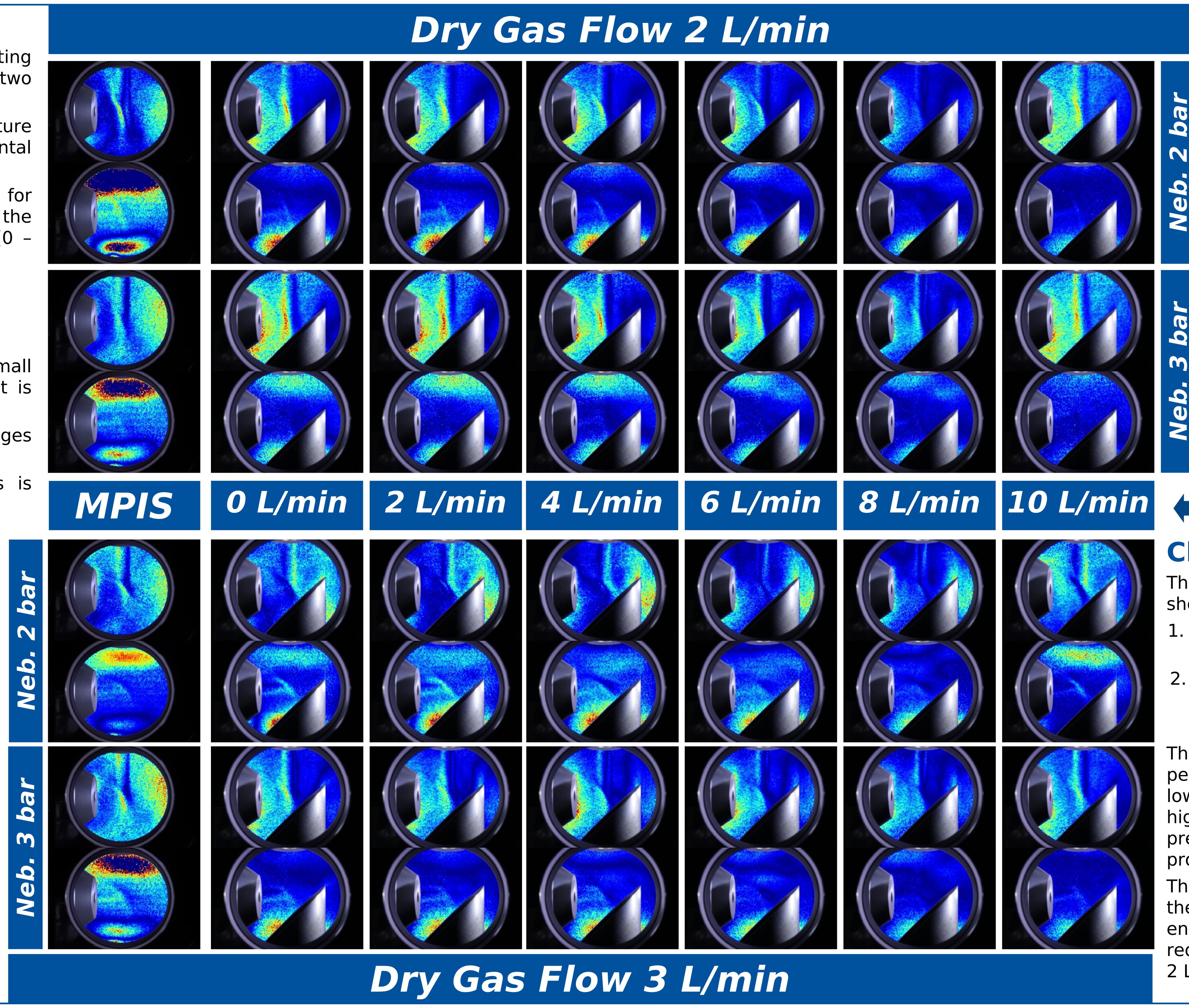
The first column shows the results obtained for the standard MPIS, the remaining columns the results obtained for the AEF configuration (0 – 10 L/min sheath gas).

1./3. row: nebulizer pressure 2 bar
All others: nebulizer pressure 3 bar

The hot dry gas caused only relatively small variations of the optical density therefore it is difficult to detect.

The nebulizer caused greater density changes and thus a greater effect.

The interaction of the different gas flows is clearly visible.



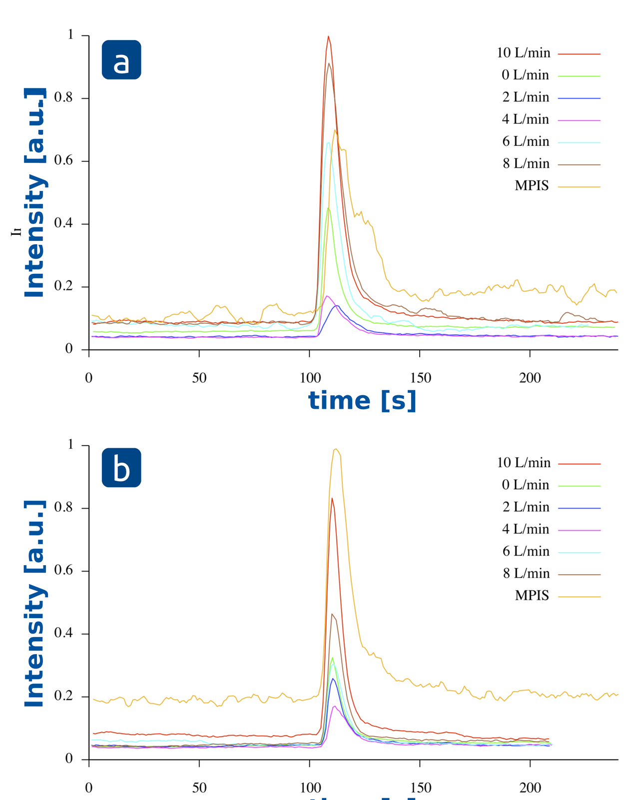
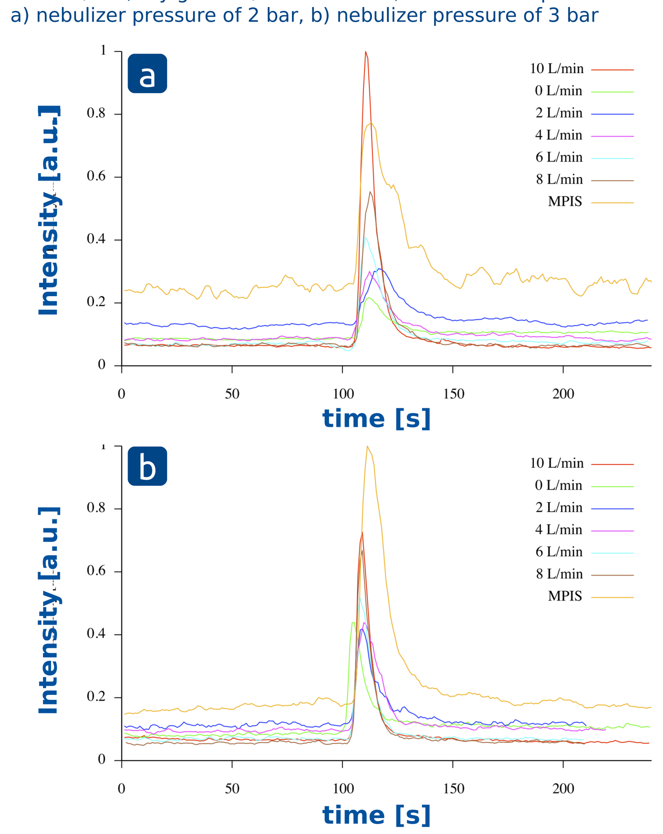


Fig. 7: Extracted ion chromatograms of pyrene, MPIS and AEF, sheath gas 0 - 10 L/min, dry gas 3 L/min at 300°C, nebulizer temperature 425°C, a) nebulizer pressure of 2 bar, b) nebulizer pressure of 3 bar

Fig. 8: Extracted ion chromatograms of pyrene, MPIS and AEF, sheath gas 0 - 10 L/min, dry gas 2 L/min at 300°C, nebulizer temperature 425°C, a) nebulizer pressure of 2 bar, b) nebulizer pressure of 3 bar



Chromatograms

The extracted ion chromatograms (figs. 7+8) show two characteristic behaviors:

1. The strong dependence of the ion signal from the nebulizer pressure
2. The non-linear influence of the sheath gas flow

The original MPIS configuration leads to wider peaks, higher background and noise ratios. At low nebulizer pressures the use of the AEF is highly beneficial. With elevated nebulizer pressures these advantages become less pronounced.

The sheath gas flow impacts on the ion signal in the following manner: Large gas flows (>6 L/min) enhance the ion signal, medium gas flows reduce the intensity more than small flows (0 – 2 L/min).

Conclusions

- The AEF changes the fluid dyna-mics of the ion source signi-ficantly
- The modified ion source leads to significantly reduced chromato-graphic peak widths due to the neutral flow optimization
- The advantages of the BOS method are demonstrated
- The experimental setup allows the visualization of different gas flows in the source enclosure
- There is no direct relation between Schlieren images and ion signal

Future Research

- AEF geometry will be further optimized
- Better visualization of the gas flows with other gases, e.g. CO_2

Literature

1)Mathias Lorenz, Klaus Brockmann, Walter Wissdorf, Dennis Klink, Oliver J. Schmitz, Thorsten Benter; Distribution of Ion Acceptance in a Fluid Dynamically Optimized Multi-purpose Ion Source, Poster TP04-068; Salt Denver, 2011. American Society for Mass Spectrometry, Proceedings of 59th ASMS Conference.

2)Thorsten Phoeler, Robert Kunte, Herwart Hoenen, Peter Jeschke, Walter Wissdorf, Thorsten Benter; Computational Fluid Dynamic Model of a Commercial Atmospheric Pressure Ion Sourc, Poster TP04-069; Salt Denver, 2011. American Society for Mass Spectrometry, Proceedings of 59th ASMS Conference.

3)H. Richard and M. Raffel; Principle and applications of the background oriented schlieren (BOS) method. Measurement Science and Technology, 12:1576-1585, 2001.

4)http://www.openpiv.net/; last visited: 04. June 2013

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