Investigation of Gas- and Ion-Dynamics in Heated Glass and Metal Inlet Capillaries: Work in progress …

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Introduction
For an optimization of inlet interfaces for API mass spectrometers, a fundamental understanding of the flow dynamics in inlet capillaries is necessary. The change of the flow conditions with the temperature is of particular interest.

State of Knowledge:
• Commonly used first gas flow restriction stages in commercial API mass spectrometers are heated, critically operated glass or metal capillaries.
• For typical glass capillaries (inner diameter: 0.5 or 0.6 mm) operated at room temperature, a number of investigations have been made, which are consistent with the assumption of a fully developed turbulent flow within the capillary.

Questions:
• Is the gas flow at higher temperatures in metal and glass capillaries comparable?
• Does the flow type, laminar or turbulent, depend on the length of the capillary?
• Are the flow conditions different at higher temperatures and smaller inner diameters?

Methods

Experimental Setup

- Within a custom ionization chamber, upstream of the capillary or inside a quartz capillary
- ATLAS H*+ emitter (248 nm)
- Anode as anolyte
- Detection: Within a custom detection chamber with a pair of electrodes mounted in parallel
- 6400 Q-Exactive Remote SourceMeter® or 617 Programmable Electrode, Keithley

Capillaries:
• In-house prepared glass capillaries (all 0.5 and 0.6 mm/length: 40–1200 mm)
• In-house prepared metal capillaries (all 0.65, 0.5, 0.7 mm/length: 40–120 mm)
• In-house prepared quartz capillaries (all 0.4 mm/length: 100 mm)

Flow Measurements:
- Ritter TG-3 Drum Type Gas flow meter or a custom homemade device

Numerical Calculations
- Comsol Multiphysics 4.4
- Data Precision 77800 Workbench (Model 53385 SP1)

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Conclusions
• The experimental setup allows measurements of pressure dependent gas flows, ion transmission and, with heating of the capillary, temperature dependence of gas flow.
• At standard conditions, the flow types of capillaries with an inner diameter of 0.4 - 0.6 mm and a length of 6 - 220 mm is in good agreement with the turbulent model data.
• For capillary lengths exceeding 500 mm, the flow characteristics at standard conditions converge for both models, turbulent and laminar. Therefore, a differentiation between both flow types can not be made.
• The flow characteristics in metal or glass capillaries are similar even at higher temperatures.
• A difference in parameters, for example, wall roughness is thus not observable.
• For higher temperatures, neither the turbulent nor the laminar model can describe the flow characteristics.
• It appears as if the models are invalid for these conditions.
• The metal capillary used in the Orbitrap mass spectrometer and the capillary used in the present setup behave differently (non-identical dimensions!)
• A clarification of the observed difference is work in progress.
• The basic numerical assessment of the capillary suggests an essentially turbulent state of the gas flow in the capillaries.

Literature
• Brockmann, K.J.; Wutz, M.; Adam, H., Theorie und Praxis der Vakuumtechnik; Vieweg+Teubner, Wiesbaden, Germany, 2011.