Novel Laminar Flow Ion Sources for LC- and GC-API MS

Ian Barnes¹; Hendrik Kersten¹; Walter Wissdorf¹; Thorsten Pöhler²; Herwart Hönen²; Sonja Klee¹; Klaus J. Brockmann¹; Thorsten Benter¹

Introduction

- Challenge: Turbulent flow, always present in classical API sources
  - Numerical simulations and experimental Particle Image Velocimetry (PIV) data show complex fluid dynamics
  - Simulation show typical Hagen-Poiseuille flow
  - Flow is determined by the MS
  - Adverse effects on reproducibility
  - Significant limitation of Dynamic Ionization Volumes (DAV) in Atmospheric Pressure Laser Ionization (APLI)
  - Alternative approach: Laminar flow API sources
    - Experiments demonstrate efficient ion transmission
    - Simulation show typical Hagen-Poiseuille flow
    - Flow is determined by the MS
    - Analyte gas phase flow is introduced in an angle of 10°
    - For APLI, laser beam is coaxially positioned
    - For APPI, radiation source is mounted perpendicularly on the tube
    - For APCI, one or two needles, are positioned in sidearms at angles of 10° to the main axis

Fluid dynamic simulations of common API sources

- Typical API source design
  - Nebulizer Gas: +0.5 – 2.0 L/min
  - Dry Gas: +0.0 – 10.0 L/min
  - Transfer Capillary: ~ 0.8 – 1.5 L/min
  - Setup dependent

- Analyte gas phase flow
  - Most stream lines “slow down” to less than 1 m/s.

Investigation of ion transport efficiencies in laminar flow tubes

- Quartz tube (40 cm)
  - Laser ionization (248 nm)
  - N/A analyte

- Analyte inlet
  - Laser beam

- Experimental setup:
  - 40 cm quartz tube, directly mounted on the transfer capillary
  - Scan of ionization positions with a 248 nm excimer laser (beam collimated to 1.5 mm cross section)

- Results:
  - 36% of signal intensity remains after 40 cm of transport
  - Investigations with metal tubes revealed comparable behavior

Simulations

- Boundary conditions:
  - Gas flow of 1.4 L/min, determined by the MS
  - Tube i.d. of 9 mm, conically shaped end with 0.8 mm orifice

- Results:
  - Typical Hagen-Poiseuille flow profile upstream of the capillary entrance region
  - Loss of ions occurs mainly by diffusion, as expected

Designs of Laminar Flow Ion Sources

Compatible analyte inlets:
- Ambient gas phase samples
- GC (in progress)
- Nano-flow LC (in progress)

Compatibility ionization methods:
- APPI
- APCI
- DA-APLI
- DA-APPI

Methods

- HPLC/Analyte: Agilent 1260
- Nebuliser: homebuilt argon spark discharge lamp
- Laser: Diode-pumped solid state laser (DSPL-532, Q-switched, 200 kHz)
- Dry gas: He, flow of 1.4 L/min, determined by the MS
- Transfer capillary: ~ 0.8 – 1.5 L/min
- Setup dependent

Literature

- Schrader, W.; Panda, S. K.; Brockmann, K. J.; Benter, Th. Characterization of laser ionization and Fourier transform ion cyclotron resonance mass spectrometry (APLI FT-ICR MS).
- Schiewek, R.; Mönnikes, R.; Wulf, V.; Gäb, S.; Brockmann, K. J.; Benter, Th.; O. J. Development of a multipurpose ion source for LC-MS and GC-API MS.
- Brockmann, K. J.; Gäb, S.; Benter, Th.; Schmitz, O. J. High sensitivity in APPI and APLI.
- Kersten, H.; Funcke, V.; Lorenz, M.; Brockmann, K.; Benter, T.; O. J. A novel ion source concept for API tandem MS.
- Schmitz, O. J. A Universal Ionization Label for the APLI-(TOF)MS Analysis of Small Molecules and Polymers.
- Constapel, M.; Schellenträger, M.; Schmitz, O. J.; Gäb, S.; Brockmann, K. J.; Benter, Th. Development of a multipurpose ion source for LC-MS and GC-API MS.