LOEWE-Schwerpunkt AmbiProbe

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN

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JOHANN WOLFGANG GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Vollantrag auf Einrichtung eines LOEWE-Schwerpunktes an der Justus-Liebig-Universität Gießen (Federführung)

„AmbiProbe – Massenspektrometrische *in-situ*-Analytik für die Problembereiche Gesundheit, Umwelt, Klima und Sicherheit“

Projekt B.1: Optimized sampling and ion transport through flexible ion guides

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Summary

Objectives: Developing ion guides and atmospheric interfaces to interconnect mass spectrometers with distant sites of ionization.
Methods: We plan to develop a helical dipole ion conduit for the transfer of monopolar ion populations, and Venturi-pump driven, fluorinated polymer device for the transfer of bipolar ion populations
Innovative Aspect:
Novel concepts for the transfer of ions at high pressures.
Relation to other Schwerpunkt-Projekten:
Devices developed within project will be used to connect ion sources developed in project A1-A3 to instruments developed in projects C1-C3

Intoduction

Although direct or ambient ionization methods allow the mass spectrometric interrogation of arbitrary samples with no sample preparation, access to point of analysis is often limited by geometric factors, i.e. sample cannot be brought to close proximity of mass spectrometer inlet, due its shape, size, weight or sensitiveness. In these cases it is highly desired to have miniaturized ion source connected to mass spectrometer through a long, ideally flexible tubing, which contains power cords and gas supply tubes for ion source and also an ion guide to transfer nascent ions to distant mass spectrometer. Generally ions can be transferred at atmospheric pressure using long flexible metal tubing, however this setup involves tremendous loss of ion current (>99.99%) and long metal tubing is not sufficiently flexible. We're planning to develop alterntives to this approach, by using RF-driven ion guides and polymer based ion transfer tubes.

Objectives

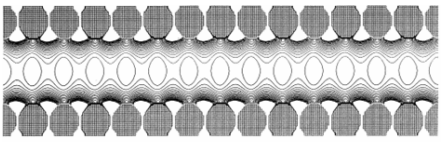
The main objective of the project is to develop ion guides which are able to transport ions at high pressures (p>1 torr) to distances in the ranges of 1-2 m, with maximum ion current loss of ~90 %. Ion guides will be based on flexible, fluorinated polymer tubing, either directly connected to fore-vacuum regime of mass spectrometer, or to Venturi air jet pump.
Further objectives include the development of optimal geometry for sampling on the distal end of ion guide, and connection to ion optics of mass spectrometer on the proximal end.
Since ionization techniques often produce multiply charged droplets and clusters, along with high amounts of solvent vapor, development of flexible heating mantle for ion guides is also planned.

Methods

We plan to develop devices for transfer of ions using flexible polymer tubing. Generally polymer tubing is inappropriate for transfer of ions due to charging effects. Inlet of polymer tubing accumulates static charges due to adsorption of ions, and this Coulombic barrier hinders ions to enter tubing. This phenomenonon will be supressed using three different strategies.
Helical dipole ion guide will be constructed by equpping flexible polymer tubing with double helix of insulated wire, and applying bipolar RF (300 kHz) onto electrodes. Resulting pseudopotential field will center the ions in the tubing, hence hinder ion adsorption on the wall. Second strategy will be to produce bipolar ion population, when opposite charges neiutralize charge build-up. Third strategy will be to increase the temperature of polymer surface, in order to shift adsorption-desorption equilibrium towards desorption. The three startegies will be used in combination to obtain optimal performance.

Preliminary results

Helical dipole ion conduit was already constructed, and preliminary data was collected using corona discharge ionization. 2 m long 1/8“ OD 1 mm ID PTFE tubing was equipped with helical electrodes, and bipolar RF was applied. The device was used as first conductance limit connecting atmospheric regime with fore vacuum region. Ion transmission efficiency of ~10 % of original atmospheric interface was achieved. It was also observed, that RF potential can be utilzed to heat the device, by choosing electrode material of appropriate resistivity.

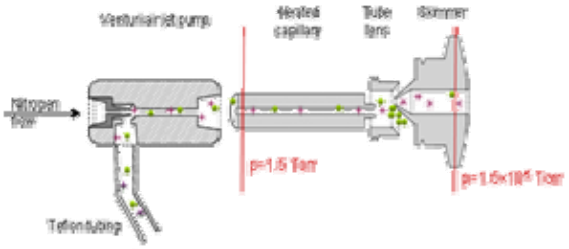


SIMION modeling of pseudopotential field in helical ion conduit

Ion sources producing ions of both polarities were combined with ion guides consisting of polymeric tubing and Venturi air pump. Using 2m 1/8“ PTFE tubing, transmission efficiency in the range of 3-5% was achived. Effect of residence time and tube length on ion survival was studied. It can be concluded, that ion recombination mainly takes place on the wall of tubing, thus combination of approach with helical dipole ion conduit or hetaing are promising approaches.

Work plan

Arbeitsprogramm:
Arbeitspaket 1: Elektrostatische und gasdynamische Berechnungen und Abschätzungen zur Ionen- und Neutralteilchen-Transmission in flexiblen Leitersystemen
Arbeitspaket 2: Entwicklung eines helikalen Druckgradient-Dipol-Ionenleiters für die optimierte Transmission in Atmosphärendruck-Massenspektrometern.
Arbeitspaket 3: Untersuchung gasdynamischer Einflüsse auf die Partikeltransmission in helikalen Dipol-Ionenleitern.
Arbeitspaket 4: Charakterisierung der entwickelten Transfereinheit hinsichtlich Massen- und Partikelgrößen-Abhängigkeit der Transmission, Teilchenladungseinflüssen und Wandmaterialeigenschaften.
Arbeitspaket 5: Einsatz des Transfersystems in kommerziellem Atmosphärendruck-Massenspektrometer für die Analytik relevanter Stoffklassen..



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