Ion chemistry simulation in Traveling Wave IMS using an open simulation framework (IDSimF)

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Introduction

Traveling wave ion mobility spectrometry (TWIMS) is an analytical method used for the separation and identification of gas-phase ions. A TWIMS device consists of a gas-filled RF-only ion guide with an additional repeating electric waveform pattern. This results in a sequence of continuously propagating potential waves along the ion guide. Ions within the device can either be swept along by the waves, traversing the drift path at wave velocity, or they can be overtaken by the waves in so-called roll-over events when they drift slower than the wave.
The ion dynamics of a reactive system within a TWIMS device is examined. This chemical system is compromised of nine water clusters in addition to nitrogen and water. A cluster of a given size can alter its size by reaction with water:

$$C_n + H_2O \overset{N_2}{\rightleftharpoons} C_{n+1}$$

The water cluster system is chosen to serve as an benchmark for the dynamics of small reactive ions in a TWIMS device in dependence of field and effective temperature.

Methods

IDSimF
The Ion Dynamics Simulation Framework (IDSimF) is an open-source software written in C++, which contains various models and modules for the simulation of ion trajectories. It provides different simulation applications, each representing a different experimental setup. Each of these applications is its own C++ program relying on several modules which provide necessary functionalities. Among them the reaction simulation module allows for the modeling of chemical kinetics and reaction dynamics via multiple different reaction types [2]. All simulations shown here were performed using IDSimF.

SIMION
SIMION was used to generate potential array files representing the electrode geometry and electric potentials for use in the simulation application [3]. A waveform profile is then applied to these potential arrays to create the transient potential wave.

The TWIMS device

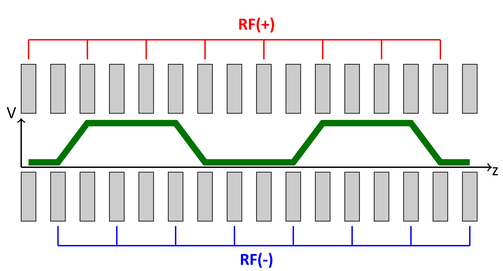

Figure 1: General structure of a TWIMS analyzer. Opposite phases of an RF-voltage are applied to adjacent electrodes in a ring electrode stack, providing radial confinement. Simultaneously, repeating waveform pattern is applied over a set amount of electrodes, yielding traveling waves which induce axial ion motion.

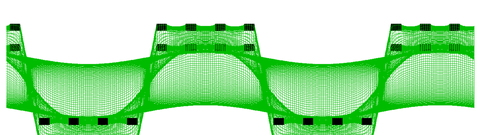

Figure 2: Potential energy surface of a TWIMS device with a repeating waveform pattern applied. In this pattern 4 electrodes are set to 0 V while the 4 following electrodes are set to 40 V.

Ion temperature

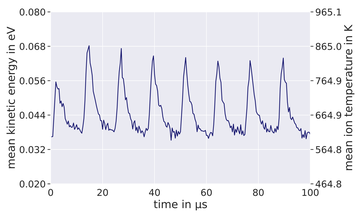

Figure 3: Mean kinetic energy and temperature for a wave frequency of 10 kHz and a water concentration of 1%.

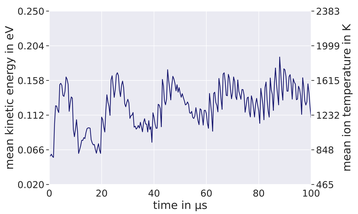

Figure 4: Mean kinetic energy and temperature for a wave frequency of 70 kHz and a water concentration of 1%.

- Figures 3 and 4 show the mean kinetic energy and ion temperature of an ensemble of 1000 particles under surfing (3) and roll-over (4) conditions
- While **surfing** a regular pattern is observed consisting of minor spikes in energy and temperature coinciding with the wave's forward stepping motion
- During **roll-over** events higher energies and temperatures can be found, however no consistent repeating pattern in the average kinetic energy due to axial diffusion of the ion cloud

Ion chemistry

Low Water Concentration (1%):

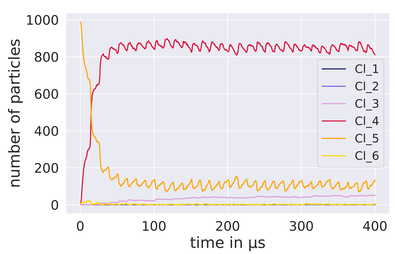

Figure 5: Particle numbers over time at 10 kHz wave frequency, water concentration 1%, wave amplitude 40 V. Starting conditions were 1000 particles of Cl_5.

- Figures 5 and 6 present the effect of the wave frequency on ion chemistry
- At low frequencies (surfing) the system quickly reaches effectively a steady state with Cl_4 and Cl_5 as the dominant species displaying minor oscillations in concentration
- At higher frequencies high ion temperatures turn the majority of particles into Cl_1 over the course of several roll-over events which proceeds to surf due its high mobility

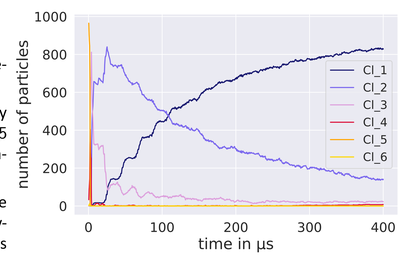

Figure 6: Particle numbers over time at 70 kHz wave frequency, water concentration 1%, wave amplitude 40 V. Starting conditions were 1000 particles of Cl_5.

High Water Concentration (10%):

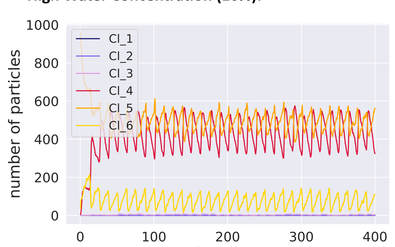

Figure 7: Particle numbers over time at 10 kHz wave frequency, water concentration 10%, wave amplitude 40 V. Starting conditions were 1000 particles of Cl_5.

- The ion chemistry was found to be dependent on the water concentration as seen in figures 7 and 8
- While surfing, an increase in the water concentration limits declustering from Cl_5 to Cl_4 and permits Cl_6 to form
- Although roll-over events still cause declustering from Cl_5 to lower weight species, higher water concentrations result in larger clusters and a wider cluster distribution

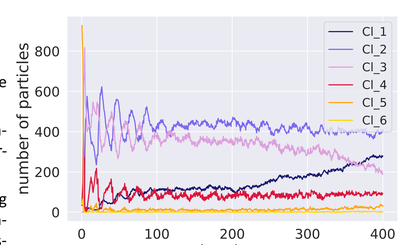

Figure 8: Particle numbers over time at 70 kHz wave frequency, water concentration 10%, wave amplitude 40 V. Starting conditions were 1000 particles of Cl_5.

Ion trajectories

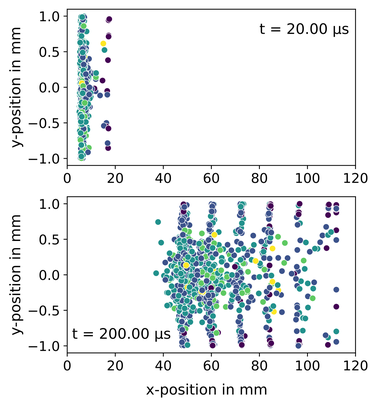

Figure 9: Scatter plots showing the positions of all particles after 20 µs and 200 µs of simulation time have passed. Axial diffusion across multiple wavesfronts is visible.

Conclusion

- We are able to accurately model the ion chemistry of a given system in a TWIMS device using the functionalities IDSimF provides
- The observed patterns in the concentrations of the cluster species can be explained based on the underlying simulated conditions
- The ion chemistry is dependent on a multitude of parameters, i.e. wave amplitude, velocity, waveform profile, concentrations, pressure

References

[1] C. Lapthorn et al., Mass Spectrometry Reviews 2013, 32, 43 - 71

[2] IDSimF; ion dynamics simulation framework; https://idsimf.readthedocs.io/en/latest/

[3] SIMION (v 8.1.2.30); ion optics and trajectory simulation program; http://simion.com/

COI Disclosure

The authors declare no competing financial interest.