Simulation of ion chemistry in Traveling Wave IMS with 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 applied 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 are slower than the wave [1].
The ion dynamics of a reactive system, consisting of nine water clusters in addition to nitrogen and water, within a TWIMS device were examined. 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 field and effective temperature dynamics of small reactive ions in a TWIMS device.

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 deliver the 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.

Results

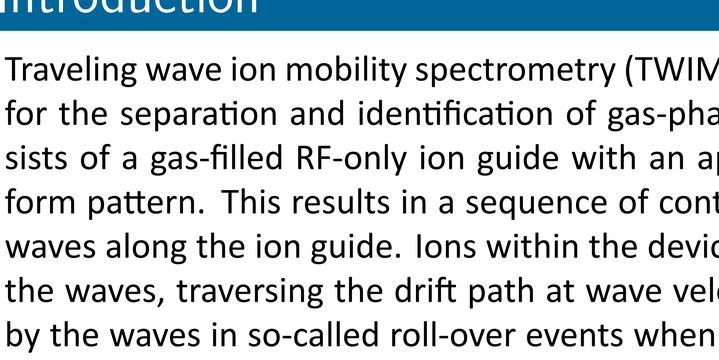

Figure 1: Mean kinetic energy and temperature for a wave frequency of 10 kHz and a water concentration of 1%.

- Figures 1 and 2 show the mean kinetic energy and ion temperature of an ensemble of 1000 particles under surfing (1) and roll-over (2) 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 repeating pattern can be established due to axial diffusion of the ion cloud

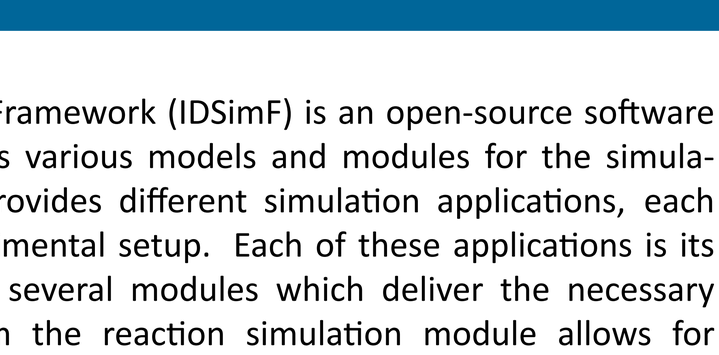

Figure 2: Mean kinetic energy and temperature for a wave frequency of 70 kHz and a water concentration of 1%.

Low Water Concentration (1%):

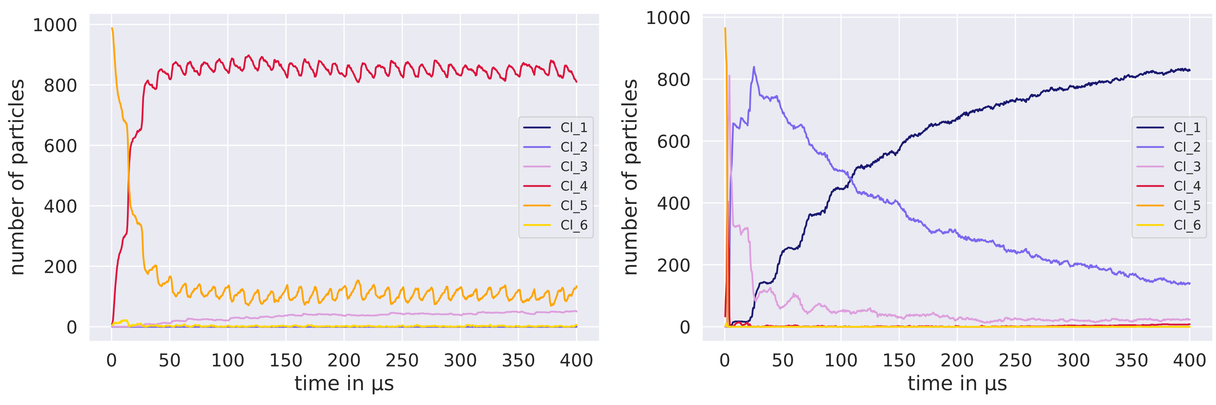

Figure 3: Particle numbers at 10 kHz (left) and 70 kHz (right) wave frequency, water concentration 1%, wave amplitude 40 V. Starting conditions were 1000 particles of Cl_5.

- Figure 3 presents the influence of the wave frequency on ion chemistry
- At low frequencies (surfing) the system quickly reaches 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, thus preventing noticeable reclustering to higher-weight species

High Water Concentration (10%):

- The ion chemistry was found to be dependent on the water concentration as seen in Figure 4
- 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 allow for a higher number of different cluster species to be maintained rather than Cl_1 quickly becoming predominant

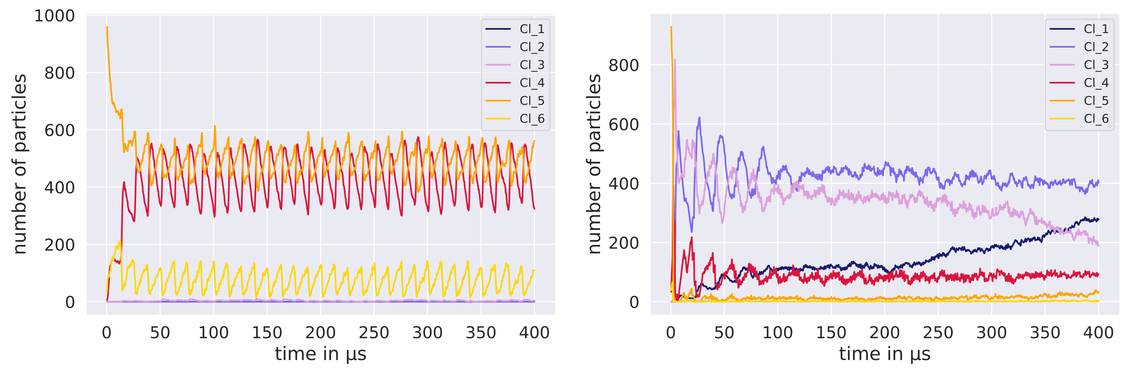

Figure 4: Particles numbers at 10 kHz (left) and 70 kHz (right) wave frequency, water concentration 10%, wave amplitude 40 V. Initial particle state: 1000 particles of Cl_5.

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/