Simulation of ion dynamics and trajectories in a Trapped IMS using an open simulation framework (IDSimF)

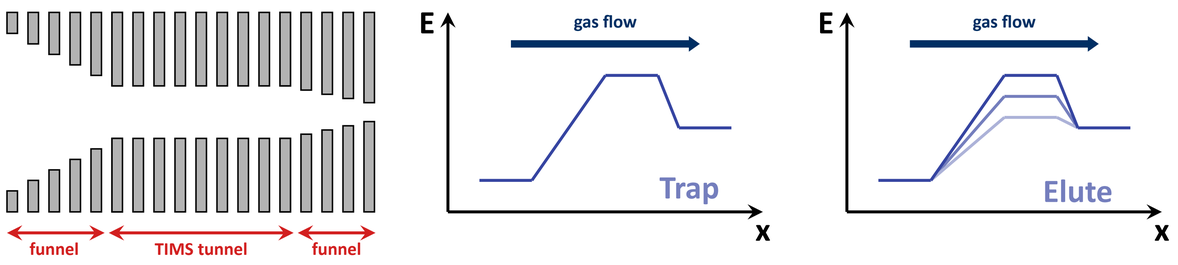
BERGISCHE UNIVERSITÄT WUPPERTAL

Physical & Theoretical Chemistry
University of Wuppertal

Maja Hammelrath*, Michelle Rajkovic, Walter Wißdorf, Thorsten Benter
*maja.hammelrath@uni-wuppertal.de

Introduction

Trapped ion mobility spectrometry (TIMS) is an analytical technique used in the separation and identification of gas-phase ions. In a TIMS device the flow of a drift gas drives ions forward while a counteracting electric field keeps them stationary. The TIMS analyzer itself is an electrode stack compromising three distinct regions: the entrance funnel, the TIMS tunnel, and the exit funnel. Radial confinement in the device is provided by an alternating RF voltage while electric field gradients are produced by superimposing DC potentials onto the RF. Ions trapped by the field are eluted by decreasing the field gradient over time.



Methods

IDSimF
The Ion Dynamics Simulation Framework (IDSimF) is an open-source software written in C++, containing 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 [1]. 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 [2]. A waveform profile is then applied to these potential arrays to create the transient potential wave.

Results

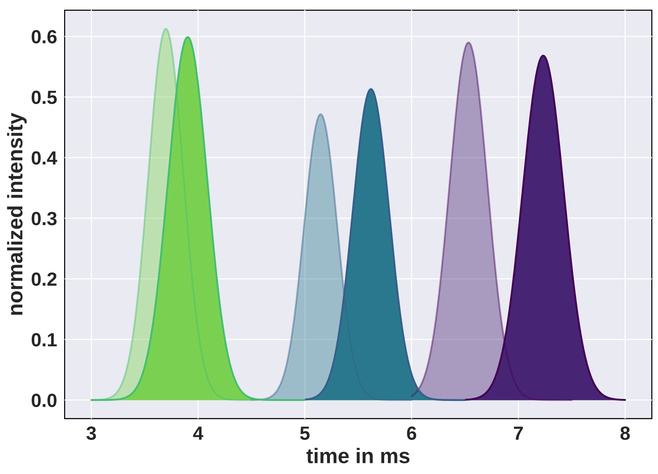


Figure 1: Arrival time distribution for the three particle groups for space charge factors of 1 (darker signals) and 100 (transparent signals). A value of 1 equates 1500 total particles whereas a factor of 100 equates 150000 total particles.

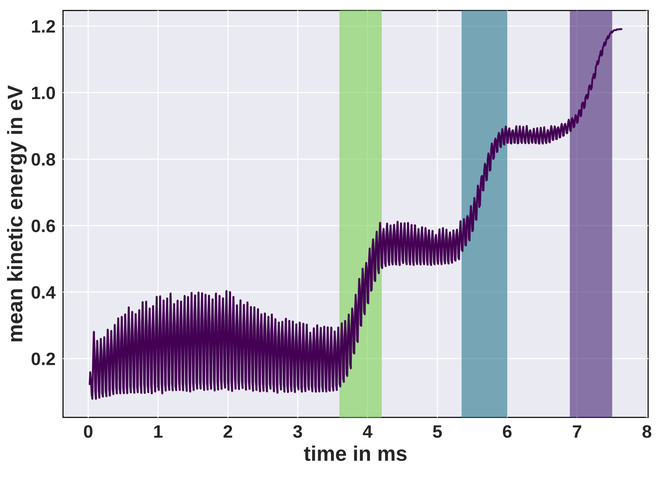


Figure 2: Mean kinetic energy across all 1500 particles over time. Three distinct steps are visible which correspond to the gradual elution of the three groups in accordance with their mobilities.

- Three hypothetical ion species were defined and used to demonstrate the simulation application

Table 1: Mass, mobility and collision diameter of the three ion species utilized in these simulations.

Species	Mass in Da	Mobility in $\frac{m^2}{Vs}$	Collision diameter in Å
1	80	2.50e-4	8.00
2	110	2.00e-4	9.00
3	140	1.50e.4	10.0

- Figure 1 and 3 show that the particles follow their expected behavior in a TIMS device, i.e. although species 3 has the lowest mobility it is the first to elute from the TIMS device
- Figure 1 presents how the number of particles influences the elution process. The peaks have shifted to lower arrival times with the effect becoming more pronounced the higher the mobility
- The mean kinetic energy of the ions over time is shown in figure 2. The constant oscillations are likely due to the confining RF field meant to inhibit the ions' radial movement.
- During elution particles are required to move up a field gradient to leave the tunnel, thus an increase in kinetic energy can be observed as the field increases

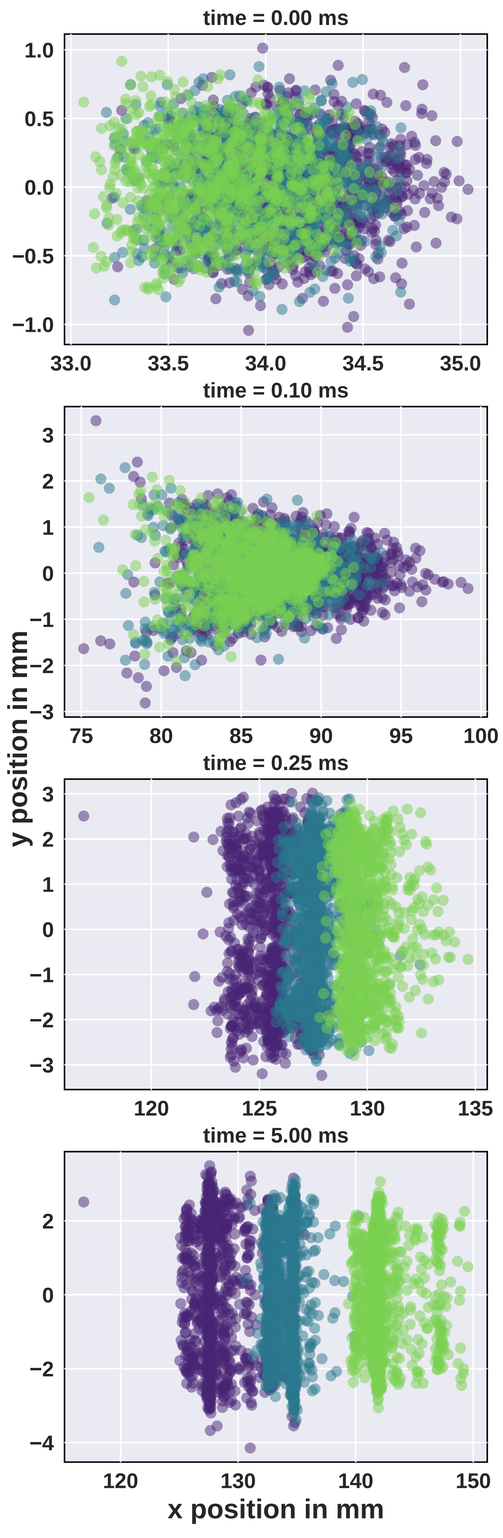


Figure 3: Scatter plot showing the positions of three different particle groups over time in the TIMS device.

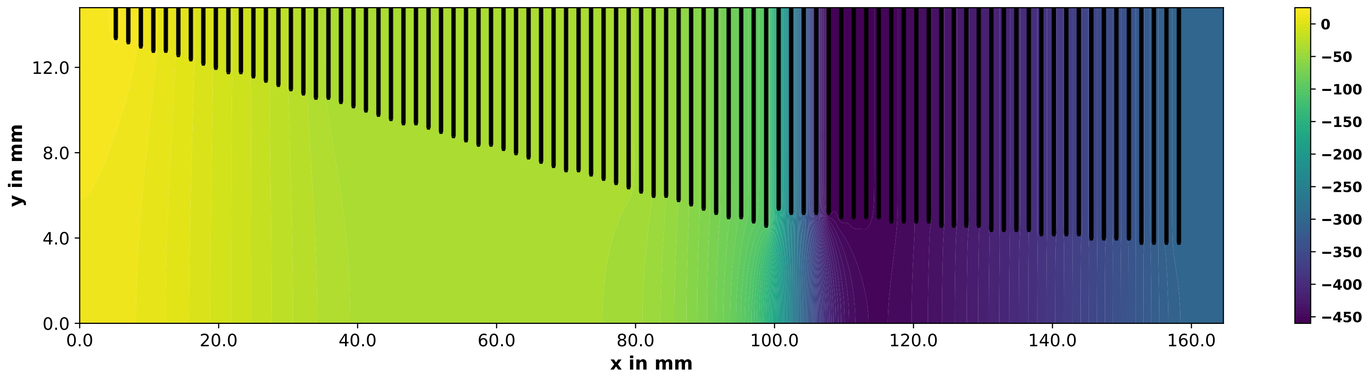


Figure 4: Calculated electric field across the TIMS device. Ions are introduced at the beginning of the Entrance funnel and moved towards the TIMS tunnel by both the gas flow and the field gradient. There they are trapped by an opposing field gradient until this gradient is reduced during the elution process.

Conclusion

- We were able to demonstrate that the TIMS simulation application is capable of accurately modeling ion behavior and trajectories
- The influence of the number of particles in the TIMS cell was shown by increasing the space charge factor

References

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

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