Comparison of Tristate Ion Shutter used in a HiKE-IMS between experimental data and simulations with IDSimF

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Introduction

High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) is a method to separate and analysis unknown substances in gas phase under vacuum conditions at 10-40 mbar[1]. The HiKE-IMS consists of a reaction tube and a drift tube. The analyte is ionized via APCI in the Reaction-tube, before it enters the drift-tube to be separate. The analyte interacts with the background gas and depending on their mobility the ions are separated. In experimental measurements it was observed that the spectra changes rapidly when high voltage was applied in the reaction region. It shows a constant high signal over the total time range, with a short break in, where the analyte is detected at low voltages. The observed phenomena also still occur after decreasing the voltage back to lower values.

Experimental Set Up

- Corona Voltage = 1,5 kV.
- reduced electric field in reaction and drift tube 80 Td.
- analyte: gas phase of pure Acetone at 40°C.

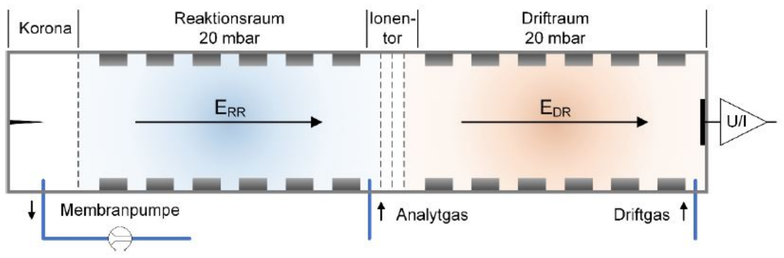

Fig. 1: Schematic overview of the HiKE-IMS. Length of reaction and drift tube is 100,5 mm and 304,5 mm[2]

Simulation

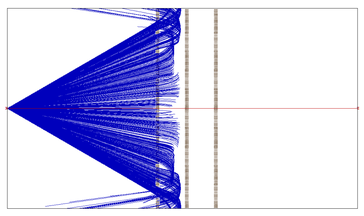

Fig. 4: Ion trajectories simulated with Simion for the close state of the Tristate Ion Shutter

- Still unclear why the signal intensity increases for high fields.
- Simion is a Software package to calculate electric fields and trajectories of charged particles.
- The Tristate Ion Shutter is implemented for the close state equivalent to 80 Td.
- the Ion trajectories in Fig. 4 shows that the ion stops at the second electrode with the maximum voltage. No ions passes the Ion shutter.

reduced field in reaction region

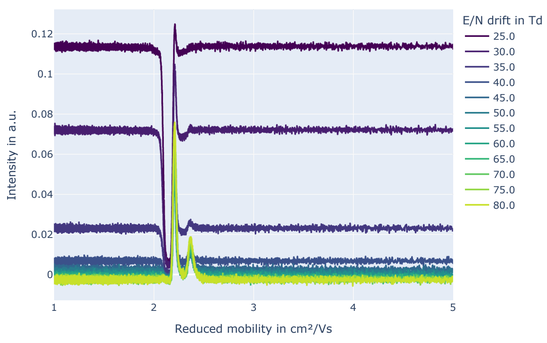

Fig. 2: variation of the reduced electric field in the reaction tube

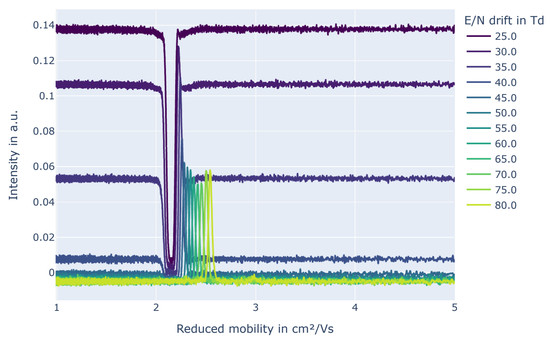

Fig. 3: variation of the reduced electric field in the drift tube

- The reduced electric field in the reaction region in Fig. 2 was varied from 25 Td to 80 Td with constant 80 Td in the drift region. In Fig. 3 the drift region was varied and the reaction region was constant at 80 Td.
- Both measurements shows a constant high signal over the total time range for low reduced fields. There is a break in in the signal intensity atshows a constant high signal over the total time range the position of the main peak.
- Variation of the reduced field in the drift region leads to a shift to lower reduced mobility. The break in also shifted to lower reduced mobility with increasing fields.
- This phenomenon only occurs after the variation of the reduced field in the reaction region and fall back to 25 Td.
- It disappeared with higher fields.
- A possible explanation is that the Tristate Ion shutter does not close totally.

Reduced Field Variation

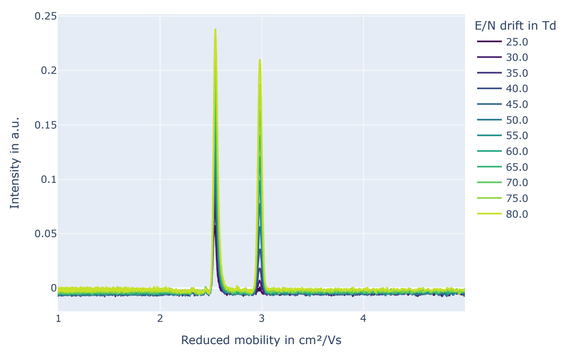

Fig. 5: variation of the reduced electric field in the reaction tube

- The reduced electric field in the reaction region was increased in 5 Td steps.
- The reduced electric field in the drift region is constantly at 80 Td.
- The intensity of both signals increases with the electric field, because more ions can enter the drift region.

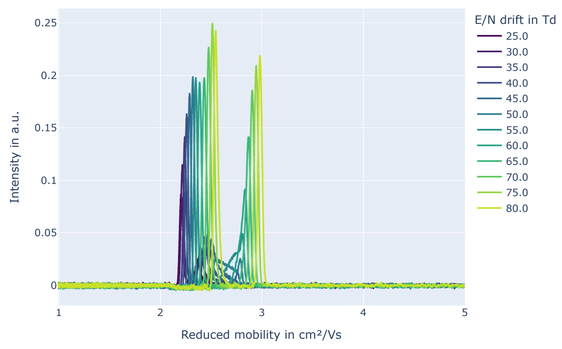

Fig. 6: variation of the reduced electric field in the drift tube

- The reduced electric field in the drift region was increased in 5 Td steps.
- The reduced electric field in the reaction region is constantly at 80 Td.
- A shift to lower reduced mobility is observed.
- Additionally it is observed that the right signal not only shifted but also broaden to lower mobility (e.g. 50 Td in Fig. 6). But the broaden signal changed his shape and indicate an Cluster transition

Conclusion and Outlook

Conclusions:

- Comparison of simulation with experimental data shows that the Ion shutter should close as expected.
- Possible transition of cluster system was observed.

Outlook:

- Optimization of the simulation for different fields and analytes.
- Measurements with different chemical systems.

Acknowledgment

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References

[1] Allers, M. et al., ”Analyzing Positive Reactant Ions in High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) by HiKE-IMS–MS”, JASMS, **2020**, Vol 31, 4, 812-821

[2] Betriebsanleitung zum Laser-HiKE-IMS