Ion Trajectory Simulation in Travelling Wave IMS with an open simulation framework (IDSimF)

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Introduction

Travelling wave ion mobility spectrometry (TWIMS) is an analytical method that allows for the separation and identification of gas-phase ions based on their mobility in a collision gas. Therein a repeating waveform pattern is applied to a gas-filled RF-only ion guide leading to a sequence of potential waves travelling along the ring-electrode stack. An ion within the TWIMS analyzer can either be swept along by the wave and display what may be seen as "surfing" behavior or the wave can pass underneath the ion in so called roll-over events. The result is a separation of ions according to their electrical mobility similar to regular drift tube IMS, although the process involves more complex molecular dynamics.

In order to examine the ion trajectories and dynamics in a TWIMS device a TWIMS simulation application is developed and added to an existing open simulation framework (IDSimF). Using this application, it is possible to examine ion drift times under varying conditions, such as different drift gases or different waveform profiles. Furthermore, detailed information about ion movement and trajectories can be acquired including ion velocities and the effective fields they experience during the wave oscillations.

Methods

The Ion Dynamics Simulation Framework (IDSimF)

The Ion Dynamics Simulation Framework (IDSimF) [1] is an open-source software, written in C++, that contains various models and programs for the simulation of ion trajectories. It provides different simulation applications modelling different experimental setups. Each of these applications is its own C++ program relying on several modules which deliver the necessary functionalities.

In order to simulate ion dynamics within a TWIMS device and thus gain insight into trajectories and drift times, an application modeling a TWIMS analyzer was developed for this framework.
To produce a pattern of potential waves with set distances traversing the analyzer, different waveform profiles in combination with phase shifts can be applied to the electrode stack by modulating the potential across adjacent electrodes.

SIMION 8.1.2.30

In order to model the electrode geometry and electric potentials, SIMION [2] is used to generate potential array files using the fast adjust option. These potential array files are then passed on to the simulation application and the waveform profiles are applied.

The TWIMS device

The simulated TWIMS device consists of a repeating pattern of 8 ring electrodes. Each electrode carries a different voltage depending on the waveform and phase shift (**Figure 1**). In addition, a confining RF voltage is applied to prevent ion loss due to radial diffusion. The electrode pattern is repeated a number of times to achieve a sufficient ion drift distance.

- Inner electrode diameter: 5 mm
- Electrode spacing: 1.5 mm
- Electrode width: 0.5 mm
- Total drift length: 112 mm
- Travelling wave amplitude: 40 V
- Confining RF amplitude: 250 V
- Confining RF frequency: 2.8 MHz

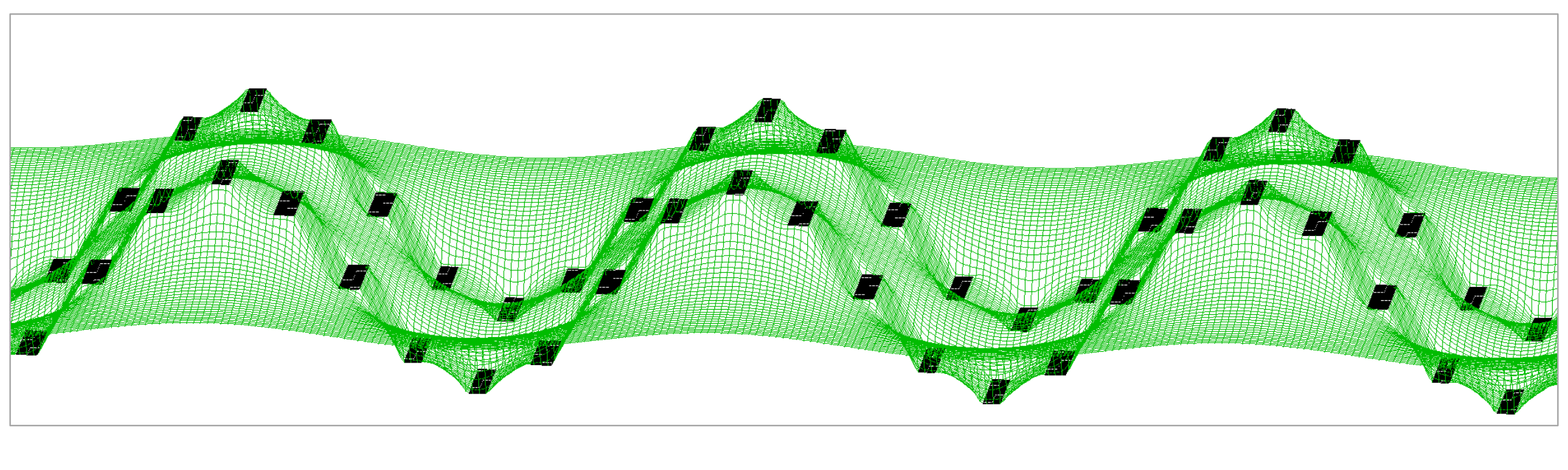

Fig. 1: Potential energy surface illustrating the travelling wave pattern

Drift time plots

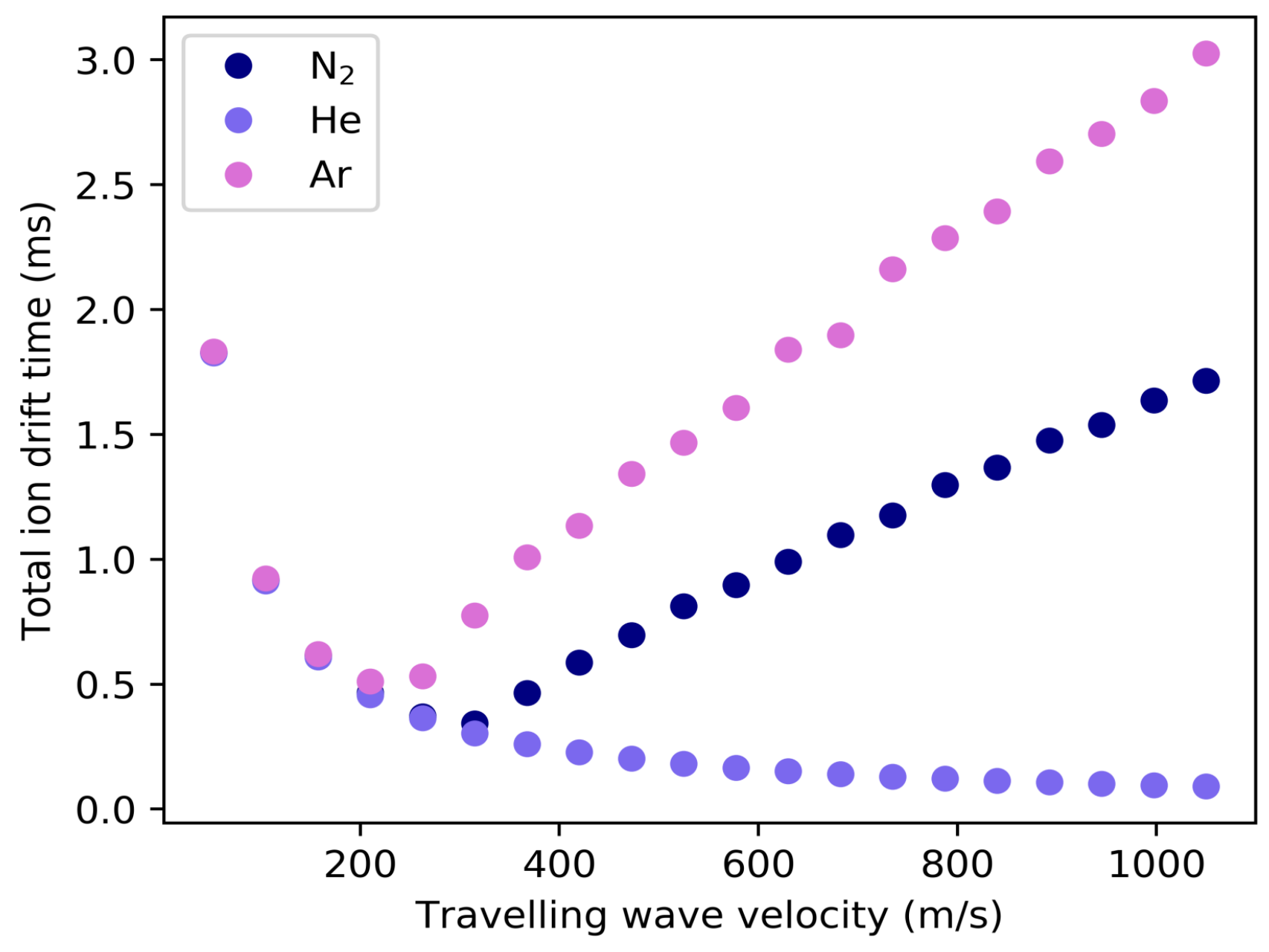

Fig. 2: Total ion drift time vs. travelling wave velocity for amphetamine ions in three different buffer gases

Figure 2 presents the total ion drift time as a function of the travelling wave velocity for three different buffer gases (Nitrogen, Argon and Helium at 2.5 mbar).

- In helium the ions consistently display surfing behavior at all velocities as ions are too fast to be overtaken
- The drift times correlate with the time it would take a single wave to pass the drift length
- In nitrogen and argon surfing behavior can only be observed at low wave velocities
- At higher velocities (above approx. 300 m/s) roll-over events start taking place.
- Generally, roll-over events start occurring at lower velocities in argon than in nitrogen due to lower ion mobility [3].

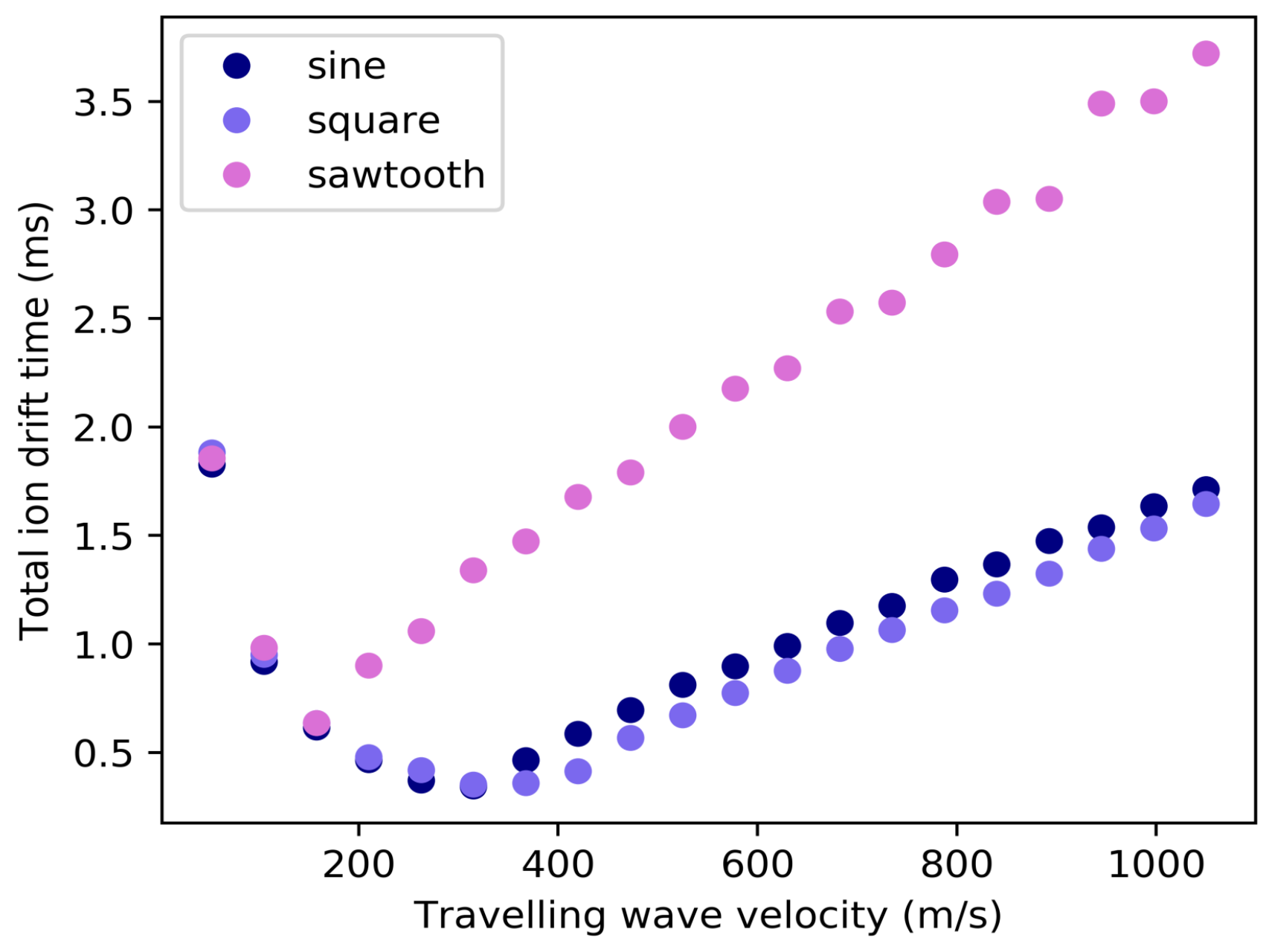

Fig. 3: Total ion drift time vs. travelling wave velocity for amphetamine ions with different waveform profiles

As with Figure 2, **Figure 3** shows the total ion drift time in relation to the travelling wave velocity for three different waveform profiles:

- Symmetrical profiles (sine & square) are fairly similar, asymmetrical (sawtooth) differs
- For symmetrical profiles, fields at wavefront and during roll-overs are of a similar magnitude
- For asymmetrical waveforms, the reverse field during roll-over events is different from the wavefront field [4]

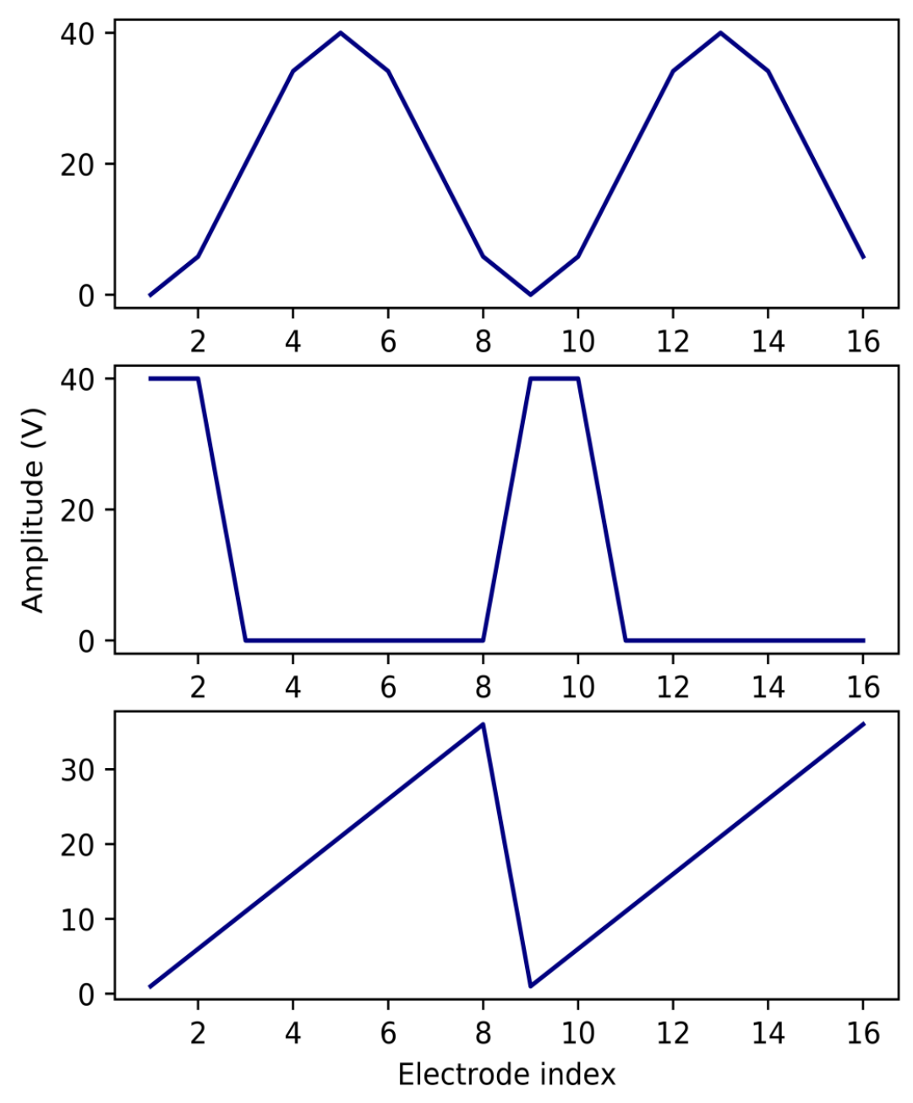

Fig. 4: Overview of different waveform profiles

Ion dynamics evaluations

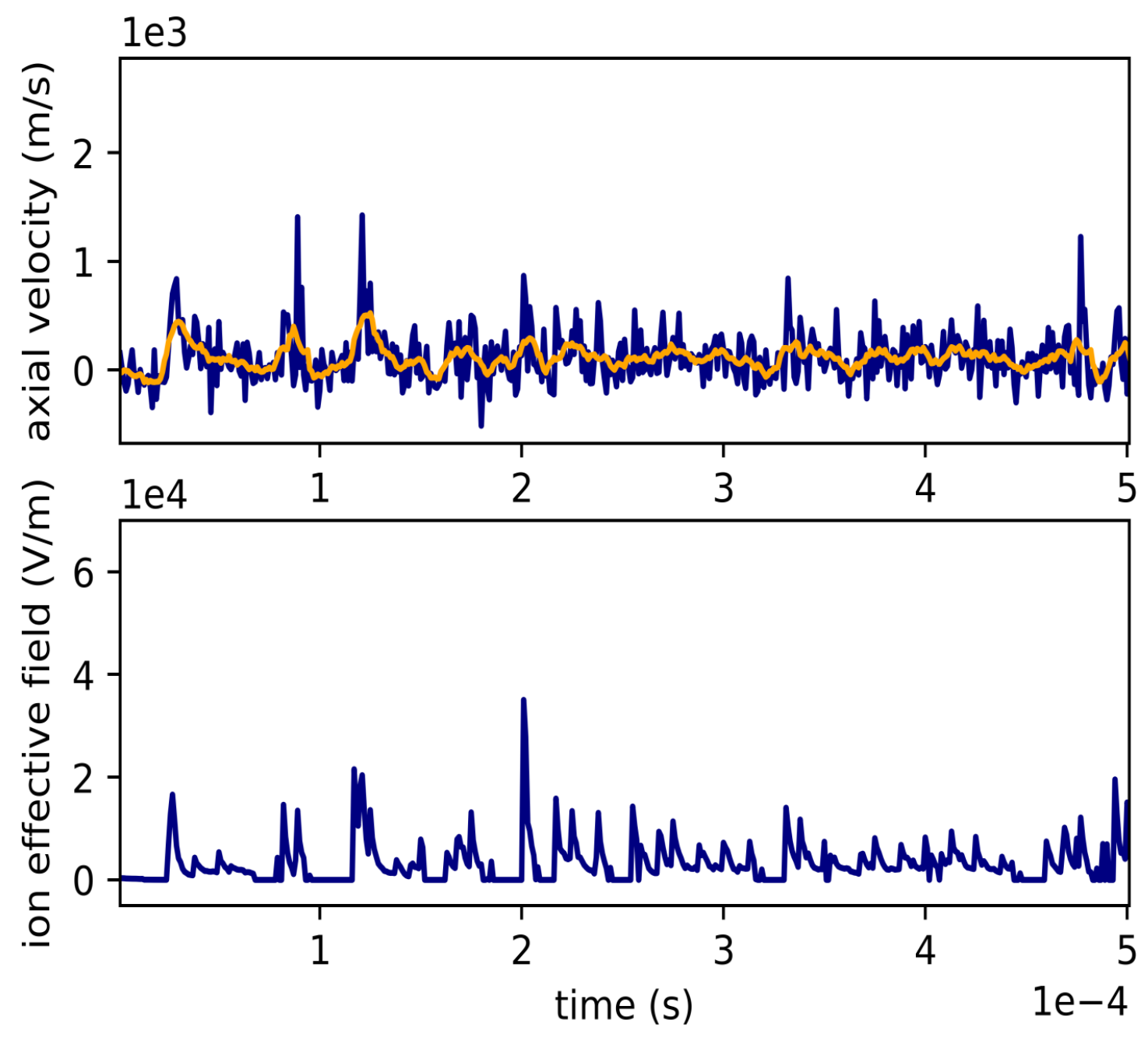

Fig. 5: Axial velocity and effective ion field over time for a single amphetamine ion in nitrogen at a wave velocity of around 100 m/s

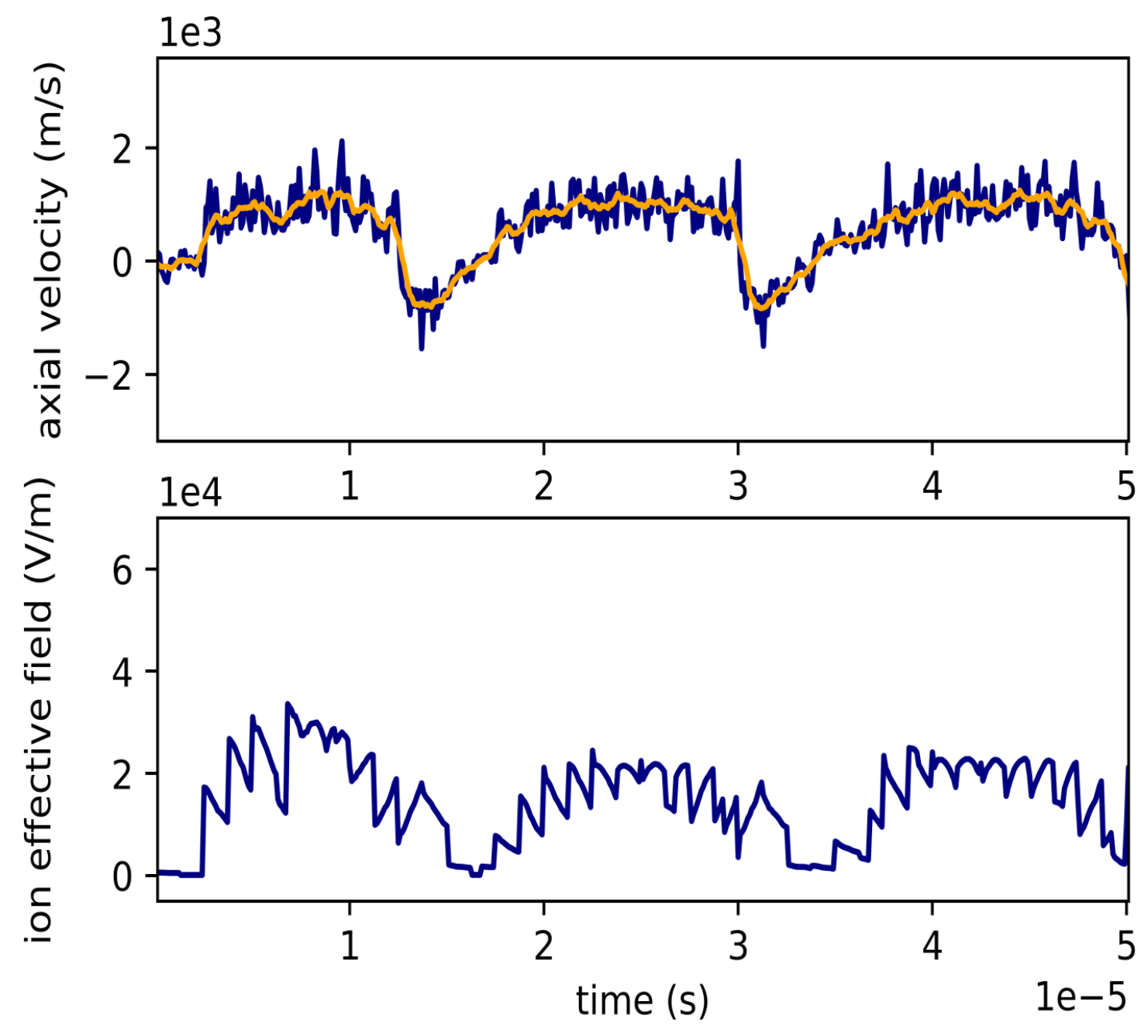

Fig. 6: Axial velocity and effective ion field over time for a single amphetamine ion in nitrogen at a wave velocity of around 1000 m/s

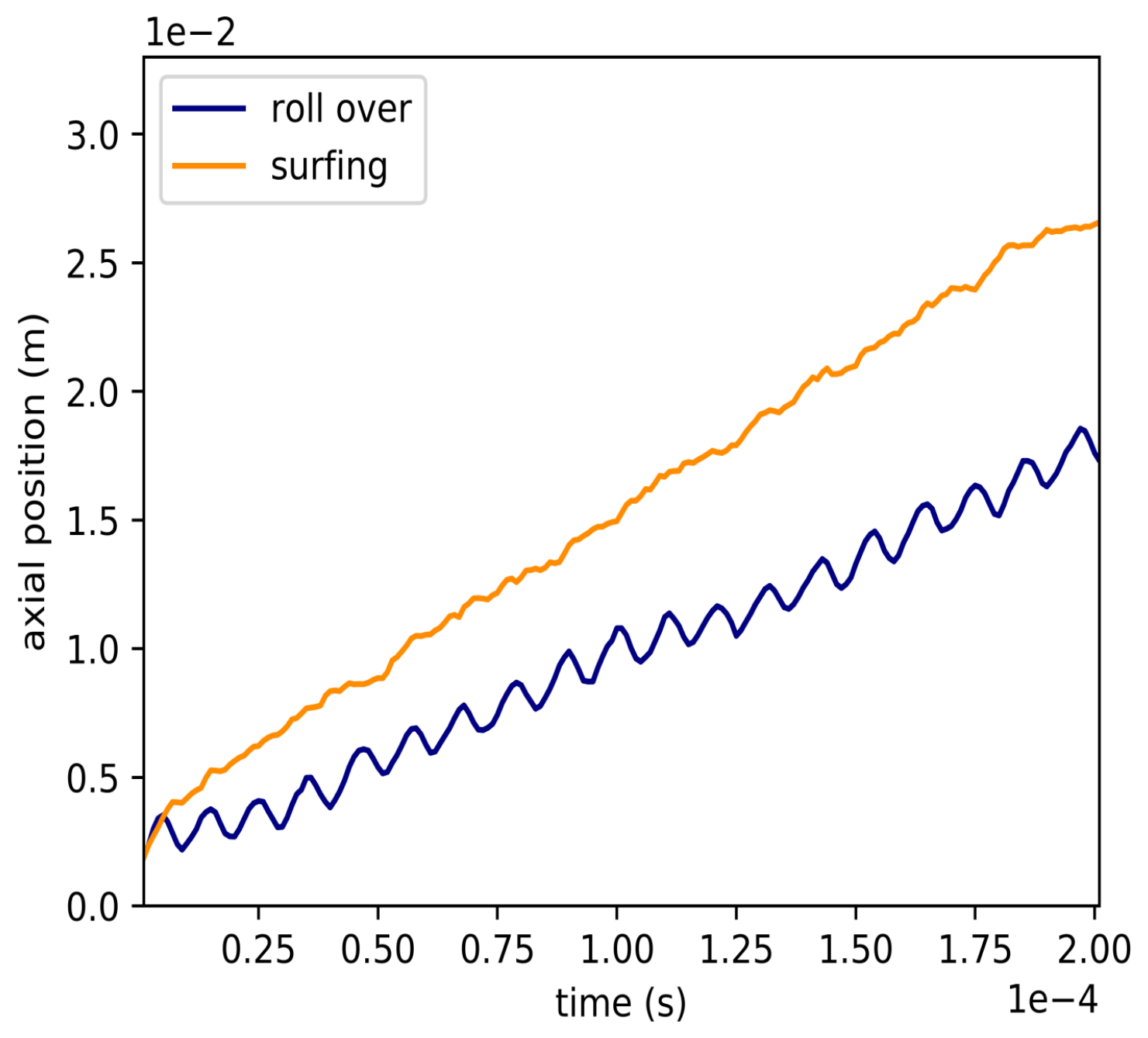

Fig. 7: Axial ion position over time for a single amphetamine ion in nitrogen at wave velocities of 200 and 1000 m/s

- **Figure 5** shows ion velocity and field for a surfing ion over the timeframe of a few waveform oscillations
- Both values remain comparatively low over time although the signal displays a fair amount of noise
- The surfing ion is not overtaken by the wave but consistently moves forward in front of it
- Therefore, no regular spikes in ion velocity and effective field can be observed

- **Figure 6** shows ion velocity and field for an ion experiencing roll-over events over the timeframe of a few waveform oscillations
- Roll-over events lead to negative axial velocities when the ion falls back down behind the wave
- Not every single passing wave will lead to an ion roll-over; an ion can temporarily ride along the crest of a passing wave before being overtaken
- Both the axial velocity and field show regular patterns

- **Figure 7** presents the change in axial ion position over time in the of both surfing and roll-over behavior
- A surfing ion displays a roughly linear increase in axial position over time as it is steadily pushed along the drift path
- An ion experiencing roll-over events shows a pattern of regular oscillations, although a net movement forward can be observed

Conclusion & Outlook

Conclusion:

- Ion drift time is dependent on the travelling wave velocity, waveform profile and buffer gas
- Ion trajectories and dynamics differ strongly depending on if the ion surfs or experiences roll-overs

Outlook:

- Use of a more refined collision model (molecular dynamics instead of hard sphere)
- Simulation of cluster systems to examine how a passing wave would influence e.g. cluster size

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/
[3] J.C. May, J.A. McLean, Int. J. Ion Mobil. Spec. 2013, 16, 85-94
[4] C.R. Conant et al., J. Am. Soc. Mass Spectrom. 2021, 32, 225-236