

# Improving ion transmission across the Funnel-SLIM interface through SIMION simulations with experimental validation



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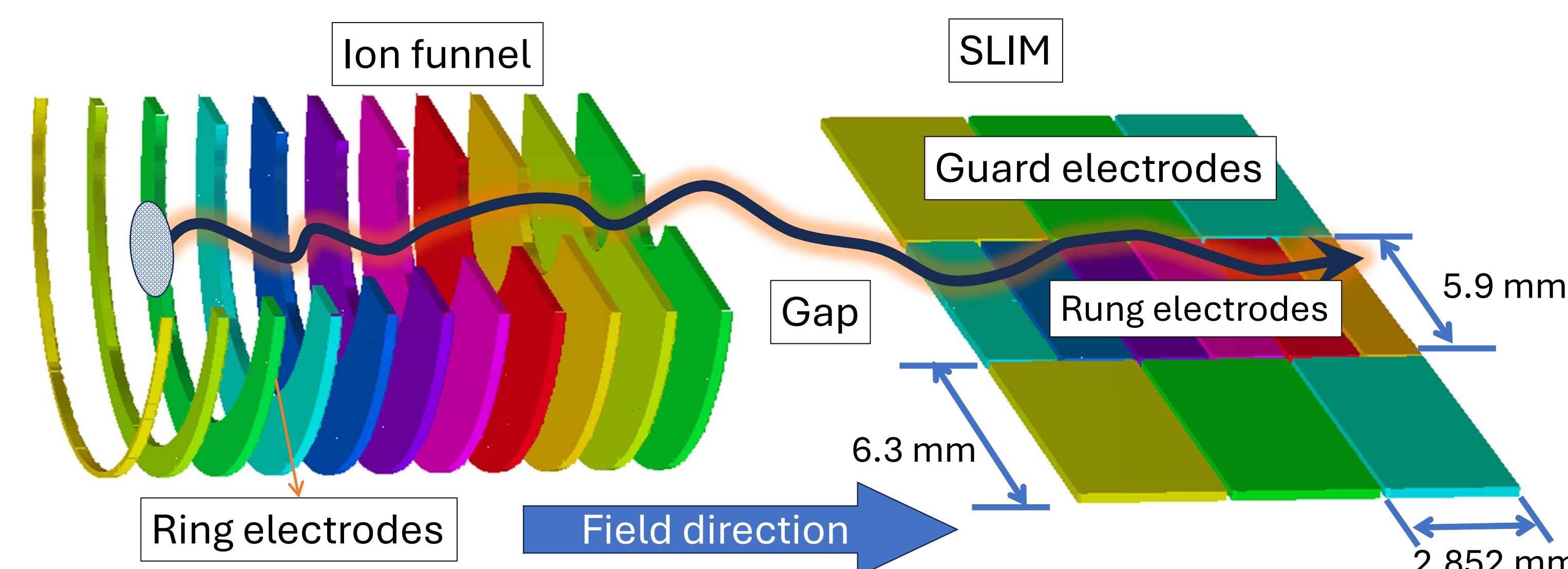
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## Introduction

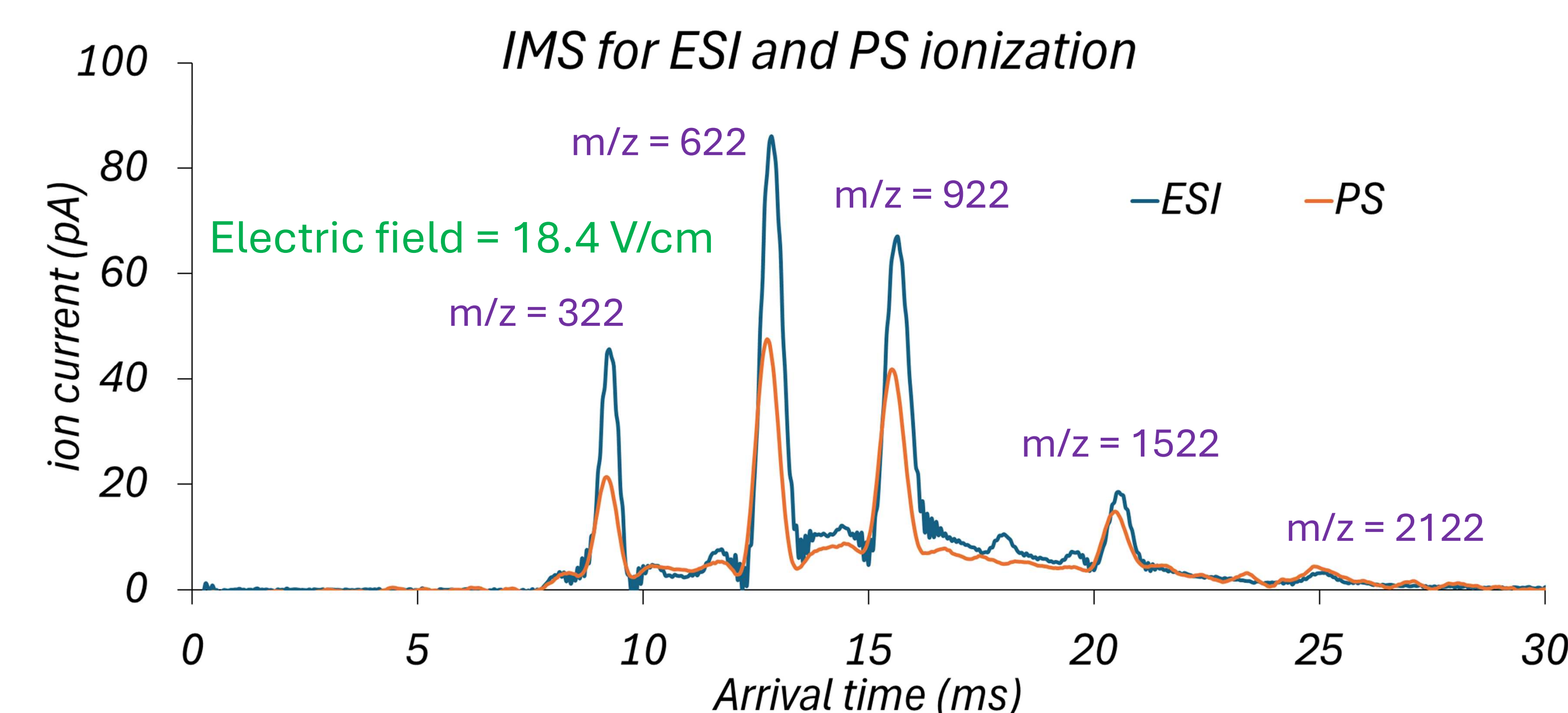
- Ion mobility spectrometry (IMS) provides structural separation of ions in the gas phase and can be coupled with mass spectrometry for complex mixture analysis.<sup>1,2</sup>
- Ambient ionization methods such as Paper Spray (PS) enable portable, direct, and rapid analysis with minimal sample preparation making IMS-MS more attractive.<sup>3</sup>
- Recently, with advancement of high-resolution IMS platforms such as Structures for Lossless Ion Manipulations (SLIM), often instrument sensitivity becomes critical, and ion losses during transfer between instrument regions can significantly reduce sensitivity.<sup>4,5</sup>
- This work investigates ion transmission across the system components, particularly funnel-IMS interface using simulations and experiments to improve injection efficiency without compromising IMS resolving power.
- We designed, built, and tested an in-house standalone ~45-cm SLIM platform, which shows a linear collision cross-section (CCS) vs. arrival-time relationship, confirming accurate, loss-free ion travel.

## Simulation setup



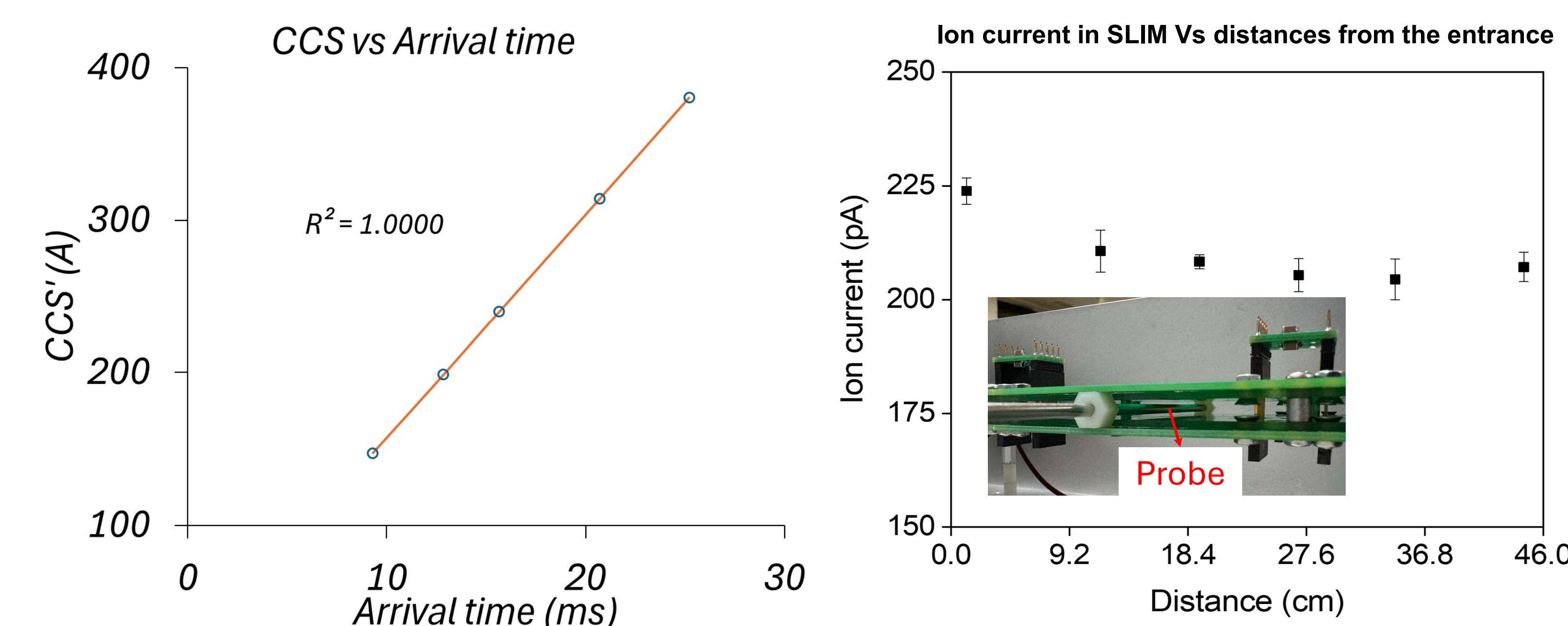
**Figure 2: Ion funnel-SLIM interface.** Ions are focused by the ion funnel and transmitted across the funnel-SLIM interface gap before entering the SLIM. Within SLIM, rung electrodes generate the drift field while guard electrodes provide lateral confinement

## Experimental Results



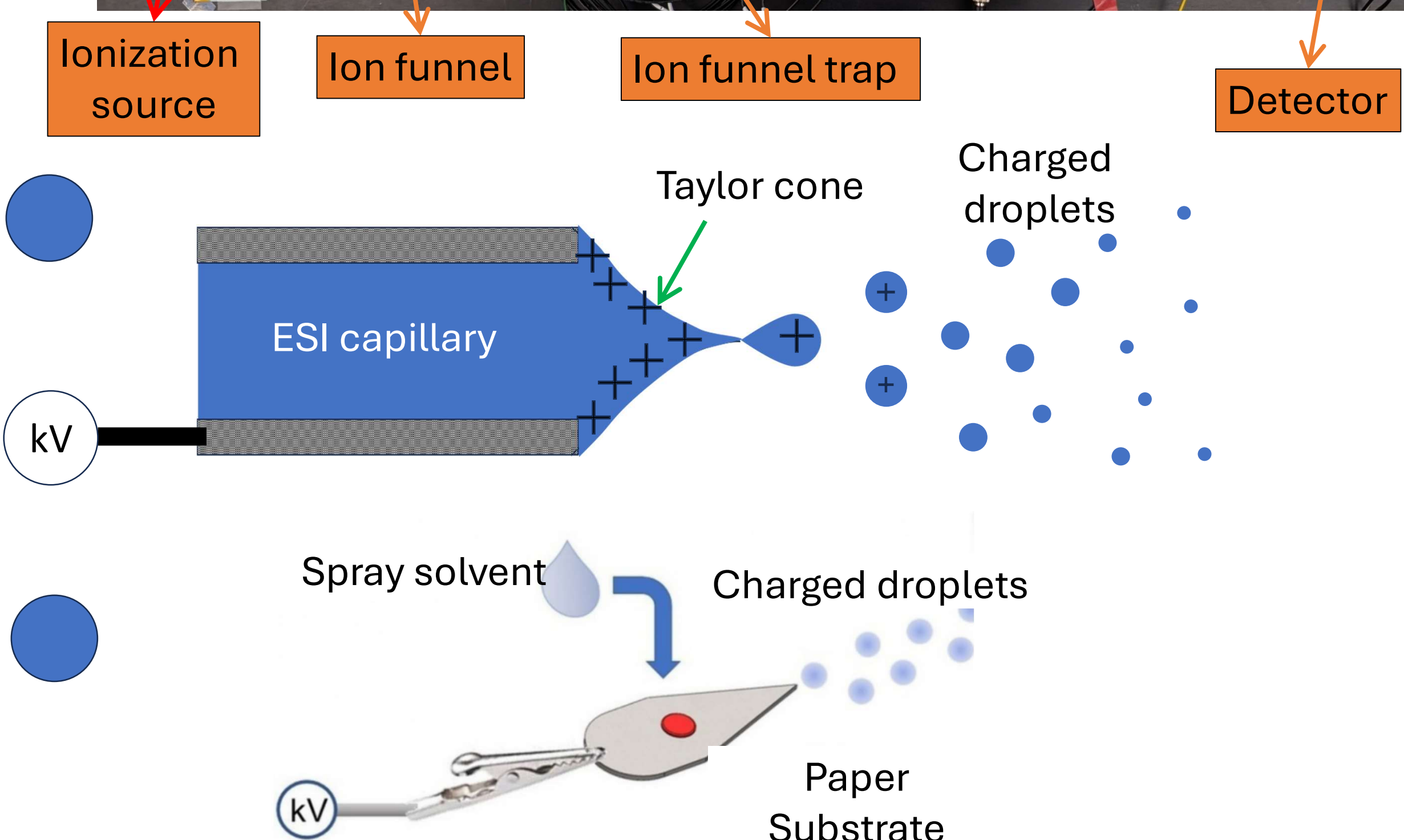
## Experimental and simulation parameters

Parameter	Value	Notes
SLIM Length (exp)	45 cm	Length of SLIM board
SLIM Length (sim)	9.14 cm	Smaller length for simulation due to computational limitations
Electric Field	From 10 V/cm to 18 V/cm	Maximum usable field strength before dielectric breakdown
Gap length (exp)	6 mm	Distance between IFT and SLIM
Gap length (sim)	1-20 mm	To check the effect of the gap distance
Gap Electric Field	Varying. See graph below	Voltage drop based on distance
Temperature/Pressure	~300 K / 4.0 Torr	Operating conditions
Ion Mixture (exp)	5 phosphazine compounds	m/z = 322, 622, 922, 1522, 2122
Ion Mixture (sim)	2 phosphazine compounds	m/z = 322, 922
Gating Time	Accumulation: 100 ms	Time for ion collection in the trap
	Trapping: 0.05 ms Release: 0.1 ms	Delay before release Time for ions to exit the trap into the drift region



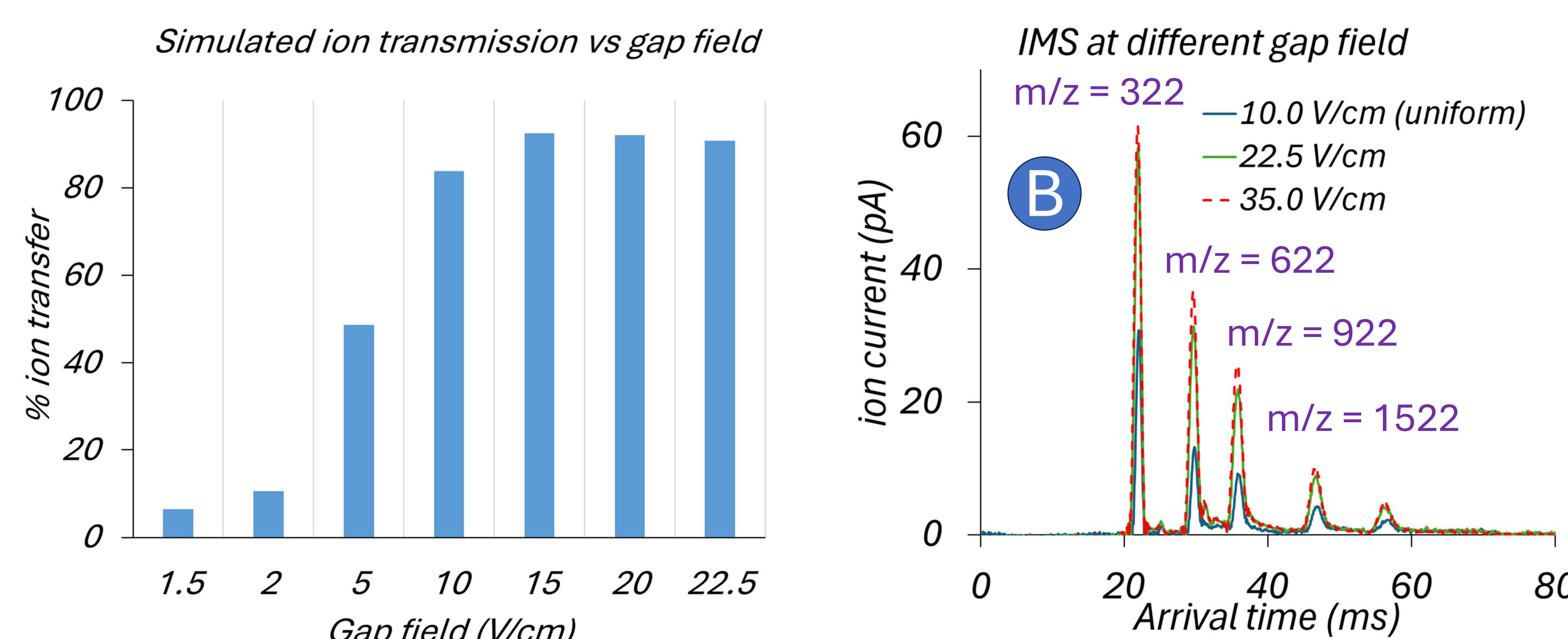
**Figure 4: Experimental IMS results at 18.4 V/cm.** Arrival time distribution with resolution of 34.5 is shown in the top figure. Linear CCS' vs. arrival time plot validates system accuracy<sup>6</sup>. Constant ion current confirms SLIM's near-lossless transmission

## Experiment setup



**Figure 1: Experimental setup and ionization methods used.** A) Ions enter, pass through the funnel and trap focusing them, before being separated across a 45 cm DC-SLIM. B) Electro spray ionization (ESI), where liquid sample is delivered through a charged capillary and introduced into the instrument as charged droplets. C) Paper spray ionization, where solvent applied to a charged paper generates droplets directly from the sample.

## Simulation results



**Figure 3: Effect of gap field on ion transmission.** A) Simulations show that increasing the electric field across the funnel-SLIM interface gap improves ion transmission. B) Experimental IMS spectra confirm higher signal at larger gap fields while maintaining resolving power.

## Conclusion and Future work

- SIMION simulations show that increasing the electric field across the gap significantly improves ion transmission, which was confirmed by experiments
- The linear CCS vs arrival time relationship validates the accuracy and resolving power of the SLIM system
- Ion current measurements along the SLIM device indicate minimal ion loss within SLIM, confirming efficient ion confinement
- Future work will focus on further interface optimization by confining the ions
- Future work also includes leaf-spray for pesticides detection

## References

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