Simulation of Differential Ion Mobility Spectrometry (DMS)

By: Francy L. Sinatra

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Background

- Radioisotope analysis is typically studied by ICP-MS or TIMS
- We are developing a lab-based DMS-MS system to assess DMS as a pre-filter for MS-based radionuclide detection
- This approach enhances the detection accuracy of the system as a result of:
  - Selection of targeted ion species before introduction in the MS
  - Provides additional orthogonal chemical information for targeted species

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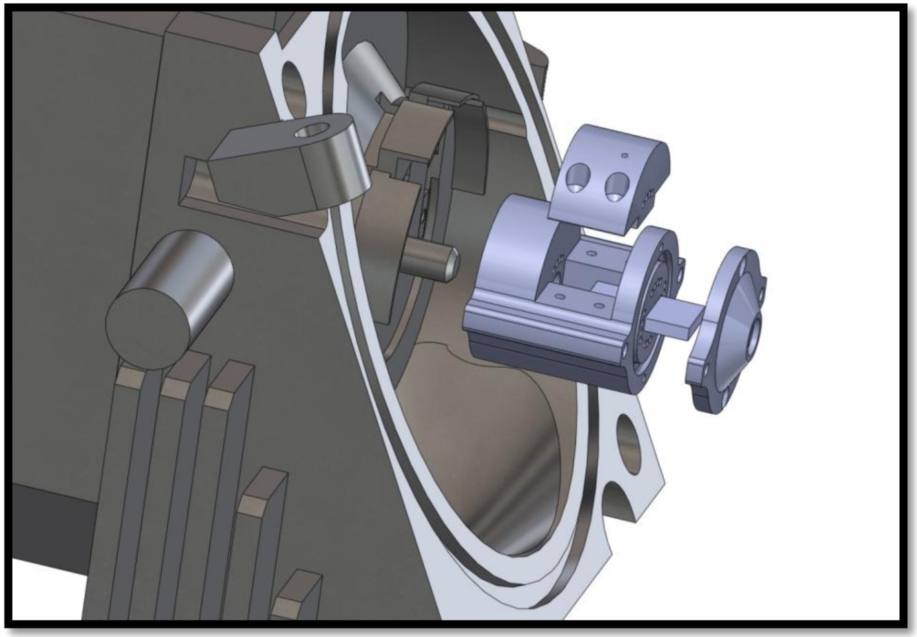
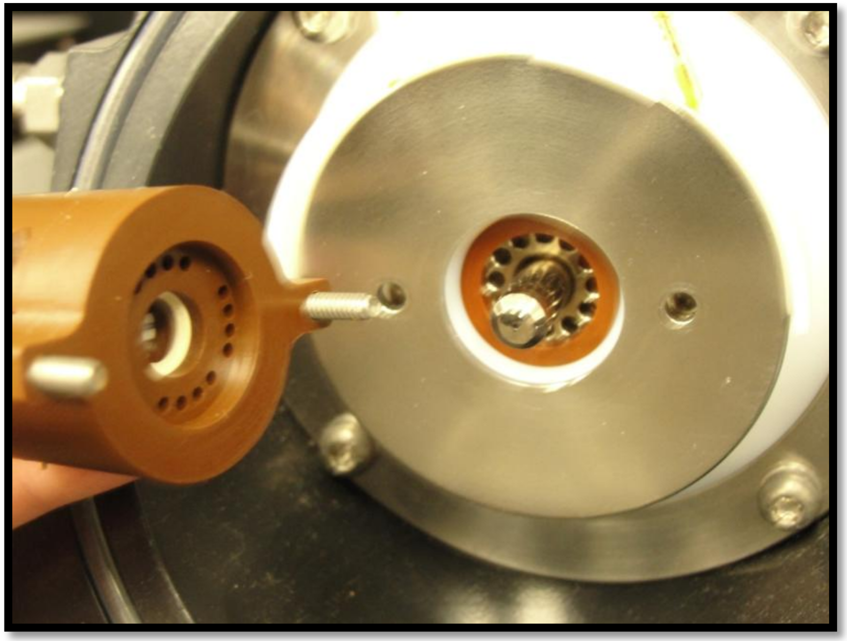
DMS / MS Design



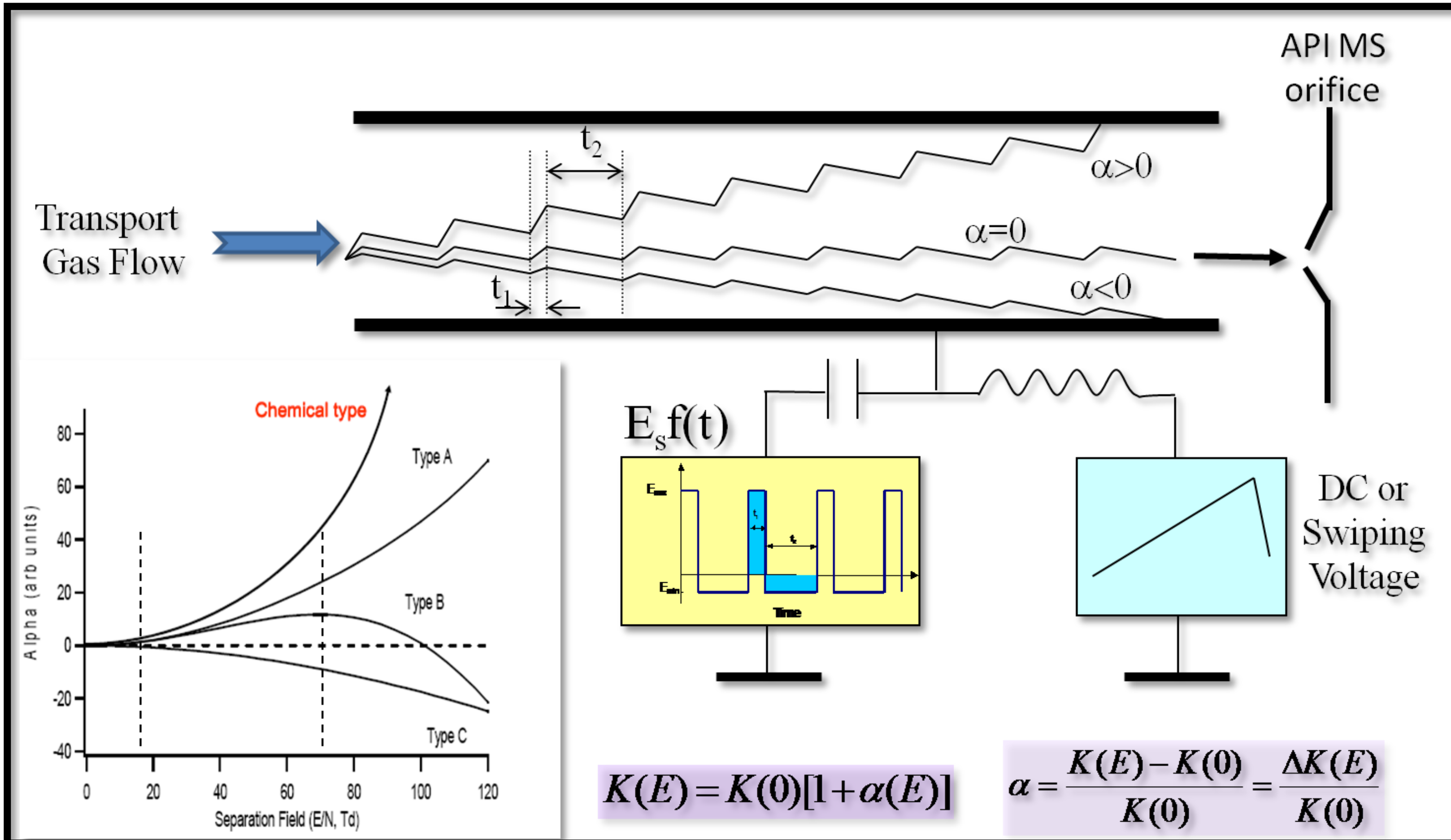


This Work

- A preliminary investigation of DMS modeling using COMSOL and SIMION software packages
  - Assessment of parameters for DMS instrumentation development such as channel length and voltage amplitude

- This work anticipates the need to optimize instrument design for maximum resolution of isobaric compounds of interest to nuclear forensic applications

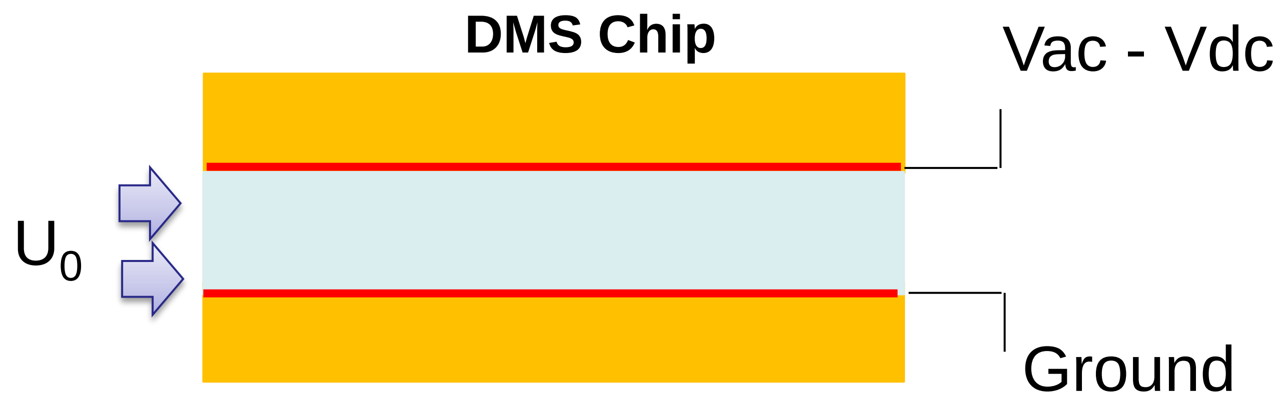
DMS Principle



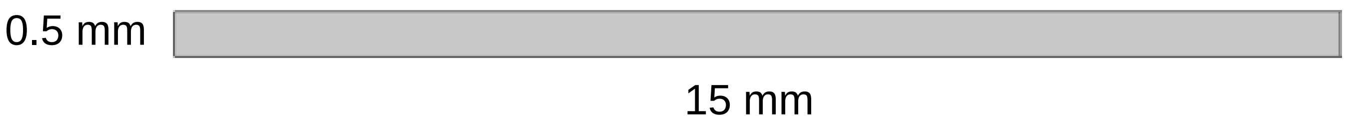
$$K(E)=K(0)[1+\alpha(E)]$$

$$\alpha=\frac{K(E)-K(0)}{K(0)}=\frac{\Delta K(E)}{K(0)}$$

Model Set-up



Medium = Air   Ions = DMMP+



Depth = 5 mm

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Model Parameters

	Parameters	Values
μ	Fluid Viscosity	1.85×10^{-5} Pa*s
ρ	Fluid Density	1.205 kg/m^3
z	Charge	1
N	Number Density (Molecules / Unit V)	$2.5e^{25}$ m^{-3}
Vdc	Compensation Voltage	-1.35
D	Diffusion Coefficient	$4.97e^{-6}$ m^2/s
K_0	Mobility for Low Electric Field	$2.425e^{-9}$ s*mol/kg
U_0	Inflow Velocity	10 m/s

Equations Used

Ion Mobility

$$K\left(\frac{E}{N}\right) = K(0)\left[1 + \alpha_2 \cdot \left(\frac{E}{N}\right)^2 + \alpha_4 \cdot \left(\frac{E}{N}\right)^4 + \cdots\right]$$

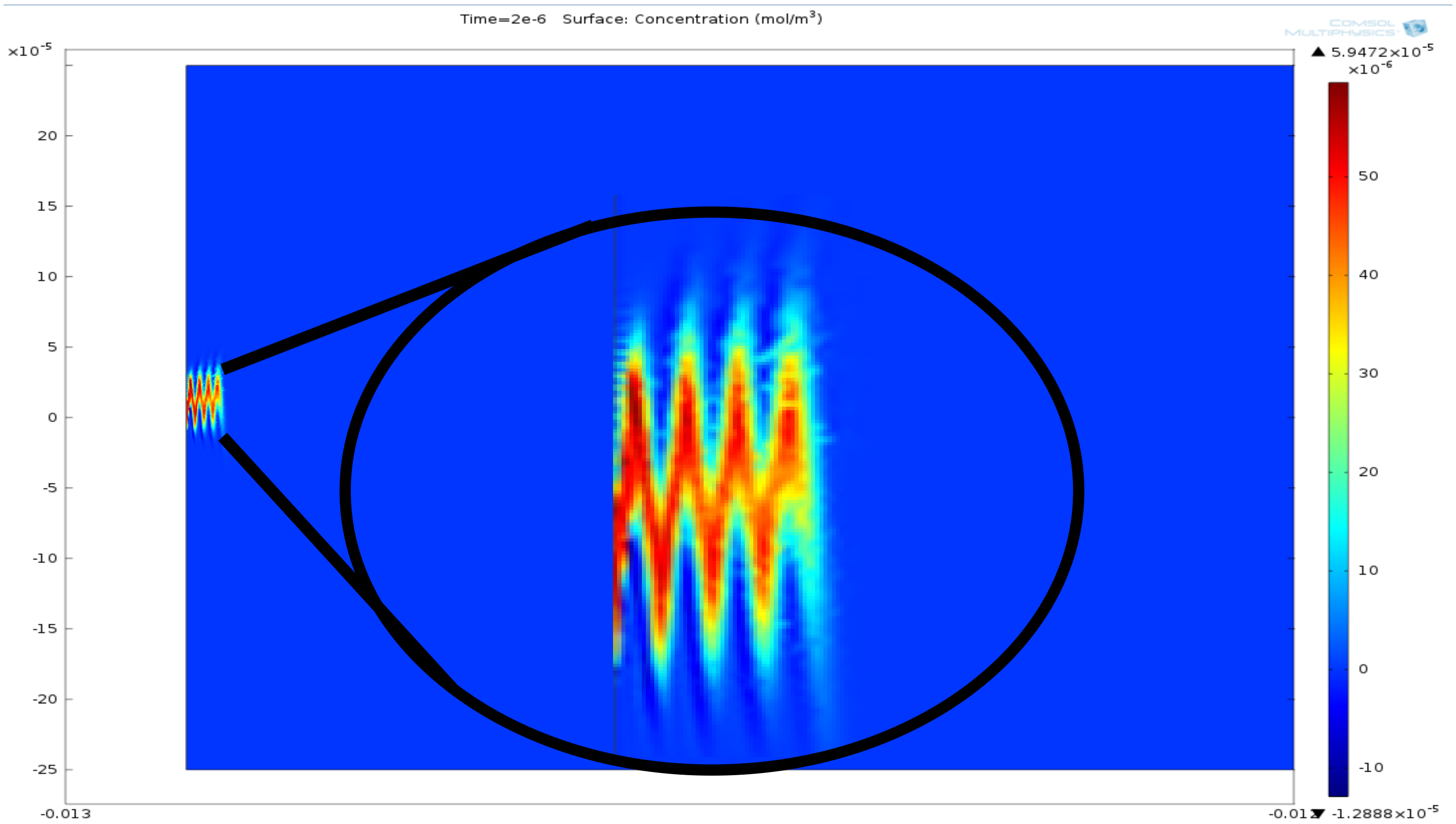
AC Voltage

$$V_D(t) = \frac{V_{iD}}{3}\left[2\sin(wt) + \sin\left(2wt - \frac{\pi}{2}\right)\right]$$

$V_{iD} = 1000$ V

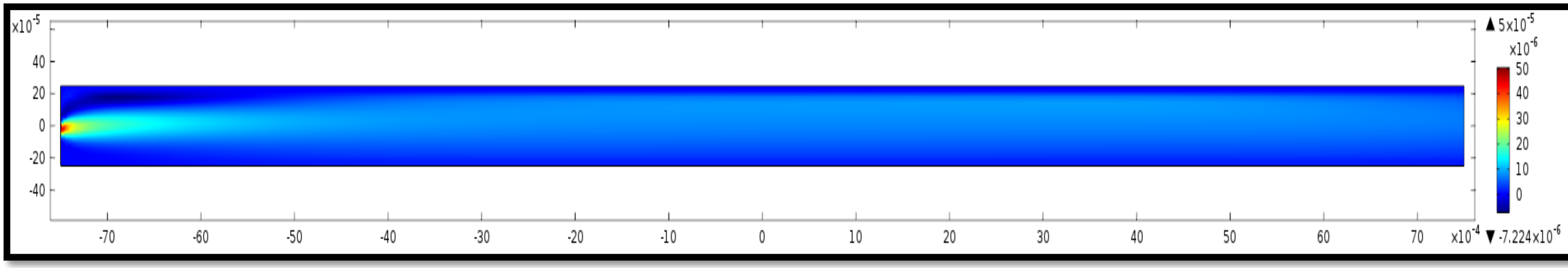
$\omega = 2$ MHz*(2π)

COMSOL – Ion Micro Oscillations



COMSOL – Ion Trajectory

DMMP+ Ions



- Carrier media is air
- Ion packets reach end of channel after 1.5 ms
- Voltage and frequency optimized for given ion species

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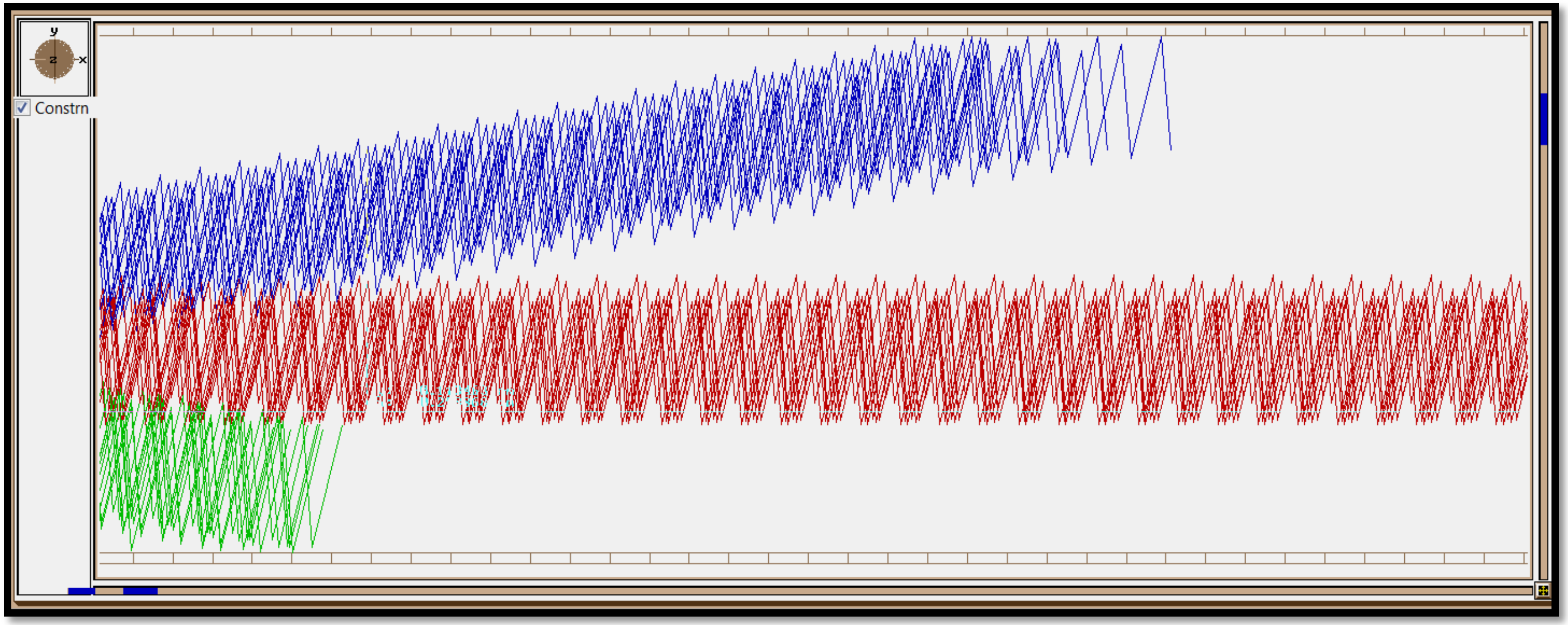
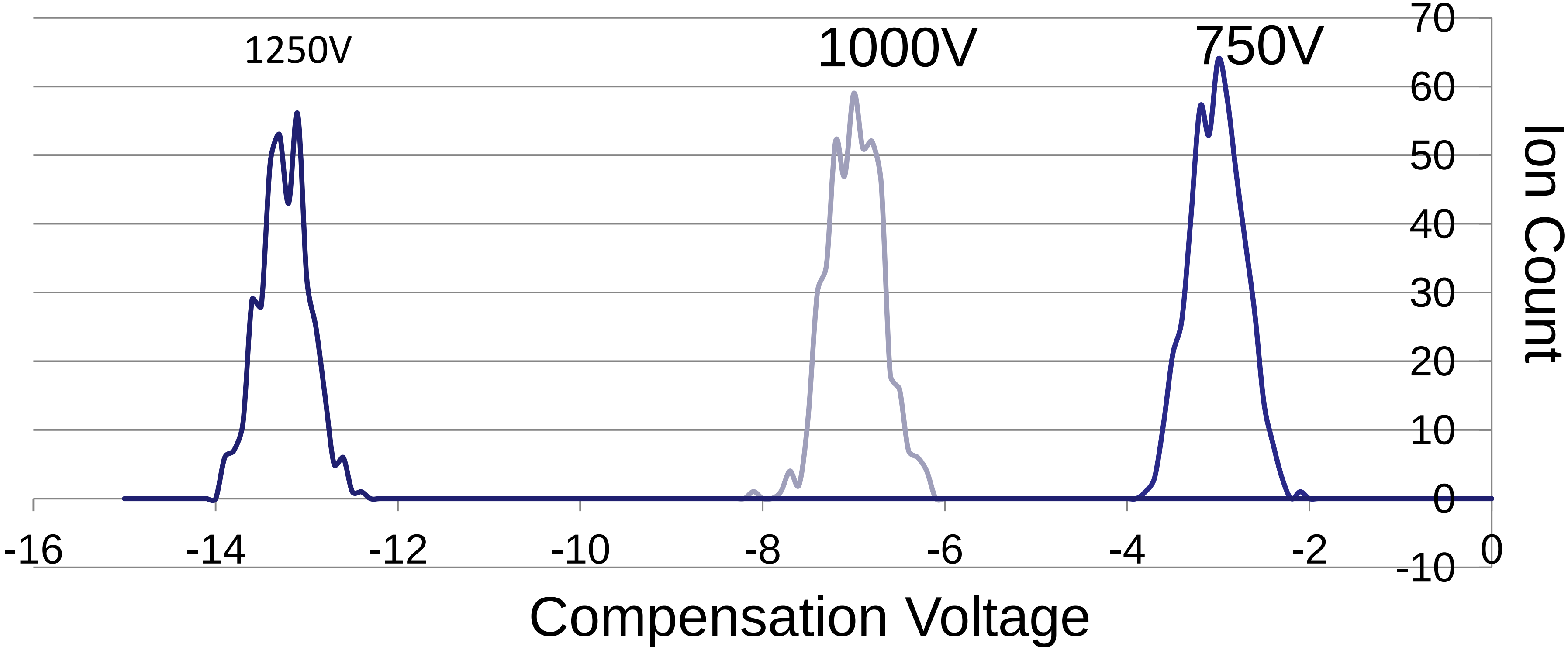
SIMION – Particle Trajectory

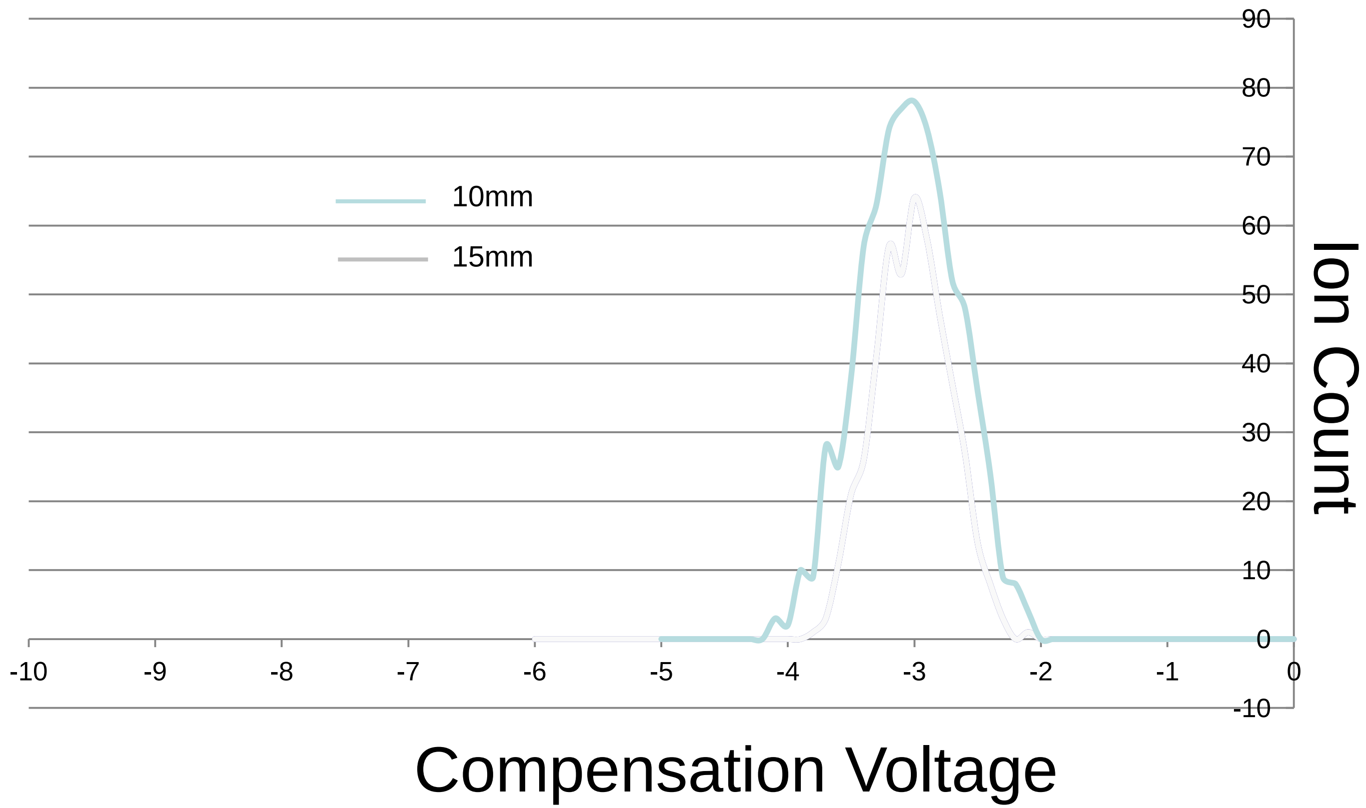


Voltage Amplitude Comparison



# of ions : 100
Mass/Charge ratio of ion: 101 ($DMMPH^+$)

Channel Length Comparison



# of ions : 100
Mass/Charge ratio of ion: 101 ($DMMPH^+$)
Voltage Amplitude 750 V

References

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