Simulation of Differential Ion Mobility Spectrometry (DMS)

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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
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
## Model Parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$ Fluid Viscosity</td>
<td>$1.85 \times 10^{-5}$ Pa*s</td>
</tr>
<tr>
<td>$\rho$ Fluid Density</td>
<td>$1.205$ kg/m³</td>
</tr>
<tr>
<td>$z$ Charge</td>
<td>$1$</td>
</tr>
<tr>
<td>$N$ Number Density (Molecules / Unit V)</td>
<td>$2.5e^{25}$ m⁻³</td>
</tr>
<tr>
<td>Vdc Compensation Voltage</td>
<td>$-1.35$</td>
</tr>
<tr>
<td>$D$ Diffusion Coefficient</td>
<td>$4.97e^{-6}$ m²/s</td>
</tr>
<tr>
<td>$K_0$ Mobility for Low Electric Field</td>
<td>$2.425e^{-9}$ s*mol/kg</td>
</tr>
<tr>
<td>$U_0$ Inflow Velocity</td>
<td>$10$ m/s</td>
</tr>
</tbody>
</table>
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

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

\[ V_{iD} = 1000 \text{ V} \]

\[ \omega = 2 \text{ MHz} \times (2\pi) \]
COMSOL – Ion Micro Oscillations
Carrier media is air

Ion packets reach end of channel after 1.5 ms

Voltage and frequency optimized for given ion species
Voltage Amplitude Comparison

# of ions: 100
Mass/Charge ratio of ion: 101 (DMMPH\(^+\))
Channel Length Comparison

Compensation Voltage

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

- http://ijims.ansci.de/pdf/9/1/Nazarov_IJIMS_9_2006_1_40_44.pdf