How Can Ion Mobility Spectrometry Separations Help your Research: Drift Tube, Differential and Traveling Wave Techniques

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In an ion mobility spectrometry experiment, a charged chemical species (ion: positive or negative) moves under a (weak or strong) (constant or varying) electrical field in the presence of a buffer gas (e.g. nitrogen, helium). Different ionic species separate based on their differences in collision cross section (CCS) or differences in ionic mobilities at low vs. high fields.
What Can Ion Mobility do for your Research?

- Increase the overall peak capacity without decreasing throughput.
- Enable detecting species with low SNR. “Clean up your spectrum”. Either in DI, UPLC or even imaging modes.
- Rapidly separate chemical compounds in mixtures based on charge state and chemical class.
- Structural tool for aiding in the determination of conformation.
- Separation of isobars with sufficiently different CCS.
- Field instrumentation (no need for vacuum).
Main Ion Mobility Techniques

- Drift tube ion mobility spectrometry (DTIMS).
- Traveling Wave Ion Mobility Spectrometry (TWIMS).
- Differential Mobility Spectrometry (DMS-planar).
- Field Asymmetric Ion Mobility Spectrometry (FAIMS-cylindrical).
- A few others (e.g., IMS-IMS, Trapped IMS) being developed and explored.
- Changing landscape….stay tuned.
Increased Peak Capacity

Peak capacity: A peak capacity of 100 tells us that 100 single-component peaks can fit into the allowed analytical dimension.

\[ \text{Total peak capacity} = \prod_{i=1}^{n} \tilde{n}_i \rightarrow \text{SCX} \times \text{RP} \times \text{DTIM} \times \text{TOF} \]

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Increased SNR

**DMS OFF**

![Graph showing m/z values and intensity for DMS OFF mode.]

- m/z 137.0255
- m/z 141.0905
- m/z 185.0737

**DMS ON**

![Graph showing m/z values and intensity for DMS ON mode.]

- m/z 137.0212

**DESI-DMS-MS in microprobe imaging mode applied to natural products on algae.**

Differential Mobility Spectrometry

• Separation based on difference in mobility at low and high field
  – Ratio of mobility at high and low field is compound-dependent
  – Related to ion clustering

Separating Compound Classes

Petroleomics

ESI-TWIMS-TOF MS

(a) \( \text{CO}_2 \) 0.70 mbar, 600m/s, 30V
(b) Gasoline with additives - ESI(-)

(c) \( \text{CO}_2 \) 0.70 mbar, 550m/s, 25V
(d) Gasoline with additives - ESI(+)


Biological Omics

MALDI-DTIM-TOF MS

Peptides (n=610)
Lipids (n=53)
Carbohydrates (n=192)
Oligonucleotides (n=96)

Traveling Wave Ion Mobility-Mass Spectrometry

\[
\Omega = \frac{(18\pi)^2}{16} \frac{ze}{(k_bT)^2} \left[ \frac{1}{m_l} + \frac{1}{m_N} \right]^{\frac{1}{2}} \frac{760}{P} \frac{T}{273.2} \frac{1}{N} \frac{t_D E}{L} 
\]

Mason-Schamp eqn. (DTIM)

\[
\Omega = \frac{(18\pi)^2}{16} \frac{ze}{(k_bT)^2} \left[ \frac{1}{m_l} + \frac{1}{m_N} \right]^{\frac{1}{2}} \frac{760}{P} \frac{T}{273.2} \frac{1}{N} A t_D^{B} 
\]

Modified calibration eqn. (TWIM)

Must use DTIM measurements to determine TWIM CCS values

\[\Omega = \text{Collision cross section}\]

\[t_D = \text{Drift time}\]

Structural MS by IM-MS

1. Background signals.
2. Other adducts.
3. Smaller MA oligomers (-1 charged).
4. Larger MA oligomers (-2/-3 charged.)
Structural MS of Metastable Oligopeptides and Oligoesters

- Molecular dynamics / simulated annealing
- MOBCAL trajectory method in N$_2$ buffer gas
- Compare computational CCS values with experimental CCS data from TWIMS-MS.

Work by Russell, Robinson, Ruotolo, Clemmer, McLean, Bush, Wysocki and many others
Separation of Isobars

\[
[C+M]^{n+} + R^- \rightarrow [C+M]^{(n-1)+} + R
\]

Figure 2. (a) Representative distributions of ion-neutral CCS values (\(\Omega\)) for FP1 and FP5 as their calcium and barium ion adducts; (b) FP1 and FP5 as the ET products of their calcium and barium ion adducts; (c) FH1 and FH2 as their calcium and barium ion adducts; and (d) FH1 and FH2 as the ET products of their calcium and barium ion adducts.
Figure 13. Schematic of GC/IMS technique, showing a $^{63}$Ni ionizer where the GC effluent is ionized, a reaction region where charge exchange takes place, a drift region where the ions are separated, and a collector where the ions are detected. The resulting ion mobility spectrum represents a plot of collector current as a function of drift time.
Looking for postdocs!
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