Transversal Modulation IMS. (TM-IMS)

“Path to next-generation IMS: new concepts, advanced instrumentation, and leveraging the ion-molecule chemistry”

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Summary

• Principle of operation:
  – One stage.
  – Higher resonances and curtain gas.
  – Two stages.

• Demonstrator TMIMS-1:
  – Architecture.
  – Resolving power.
  – Robustness

• Demonstrator TMIMS-2:
  – Architecture.
  – Background reduction.
  – IMS-IMS analysis.

• Numerical simulations.

• Conclusions.
Principle of operation: One stage.

- Ideal uniform electric fields:
  - Velocity trajectories:
    \[
    u = KE_0 \\
    v = KE_1 \sin(\Omega t)
    \]
    \[
    x = KE_0 (t - t_0) \\
    y = 2 \frac{KE_1}{\Omega} \sin \left( \frac{\Omega}{2} (t - t_0) \right) \sin \left( \frac{\Omega}{2} (t + t_0) \right)
    \]
  - Distance to the outlet slit
    \[
    Y = 2 \frac{KE_1}{\Omega} \sin \left( \frac{\Omega l}{2KE_0} \right) \sin \left( \Omega t - \frac{\Omega l}{2KE_0} \right)
    \]
  - Selection criterion:
    \[
    K' = \frac{\Omega l}{2\pi E_0}
    \]
Principle of operation: Higher resonances.

- Resonant mobilities:
  \[ K_n = \frac{\Omega l}{2n\pi E_0} \]

- Curtain gas in the inlet slit acts as high mobility pass filter:
  - sweeps away low mobility ions and prevents agglomeration of resonant peaks.
- Resolving power of the high pass filter \( R > 2 \) is enough to separate \( K_1 \) and \( K_2 = K_1/2 \).
Principle of operation: Two stages.

• One stage produces a pulsed output of non desired ions:

\[ Y = 2 \frac{KE_1}{\Omega} \sin \left( \frac{\Omega t}{2KE_0} \right) \sin \left( \Omega t - \frac{\Omega t}{2KE_0} \right) = 0 \]

• Two stages operated in quadrature (same frequency) eliminate the pulsed output.

• Each stage can be operated with a different gas and a different voltage
  — **IMS-IMS analysis.**
**TMIMS-1: Architecture.**

- One single stage.
- Nano-ESI ion source
- Electrometer detector
- IMS analysis

TMIMS-1: Resolving power (Res).

Theoretical estimation

- Ions spread due to diffusion.
  \[ \sigma^2_r = 2D\tau \]
- Calculate instantaneous signal \( N(Y, \sigma_r) \)
  \[ S = \frac{1}{\sqrt{2\pi\sigma_r}} e^{-\frac{1}{2\sigma_r^2}} \]
- Integrated averaged signal.
  \[ \bar{S} = \int_0^{2\pi} e^{-\frac{1}{2}\left(\frac{E_1}{E_0} - 1\right)^2} A\sin^2(\theta) d\theta \]
- Reconstruct spectrum, FWHH.
  \[ R_D \approx 0.187 \frac{E_1}{E_0} \sqrt{\frac{V_0e}{k_B T}} \]

Experimental results

- \( Res \) grows with the square root of the axial voltage.
- \( Res \) grows with the deflector voltage until trajectories collide with deflector electrodes.

![Graphs showing theoretical and experimental results](image-url)
**TMIMS-1: Robustness.**

- Electronic alignment compensates for mechanical misalignments.
  - Tolerates mechanical misalignments as high as 1mm.
  - Tolerates 5V error in mean deflector voltage.

- Transversal voltage: circles
- Longitudinal voltage: squares
- Different wave amplitude voltages: diamonds
TMIMS-2: Architecture.

- Two stages.
- Two gases.
- Nano-ESI ion source
- Electrometer detector
- IMS and IMS\(^2\) analysis
**TMIMS-2:** Background reduction.

- Synchronization of Stages eliminates pulsed signals

![Graph](image)
TMIMS-2: IMS\textsuperscript{2}

- ESI: MeOH, H2O, THABr.
- Stage 1: N\textsubscript{2}
- Stage 2: N\textsubscript{2} with 1\% iso-propanol.

- ESI: MeOH, H2O, HCl, PETN
- Stage 1: CO\textsubscript{2}
- Stage 2: N\textsubscript{2}
Numerical simulations:

- Allow us to simulate real geometries.
  - Electric fields: Boundary Element Method.
  - Ideal convective trajectories: Runge-Kutta.
  - Diffusive model: Transversal diffusion $\sigma^2 = 2D\tau$
- Validated with TMIMS-1 and TMIMS-2.
- Used to determine optimum geometries
Conclusions

- Transversal Modulation IMS (TM-IMS) works.
- Resolving power: R=55
- Very robust.
- Duty cycle: 100%
- True mobility
- Inlet and outlet are very accessible.
- Allows IMS, IMS$^2$ and can be deactivated.
- Operates at atmospheric pressure
  - Upstream the orifice plate.
  - Allows easy upgrading of current API-MS
- Good candidate for IMS-MS applications.
Thanks for your attention!

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