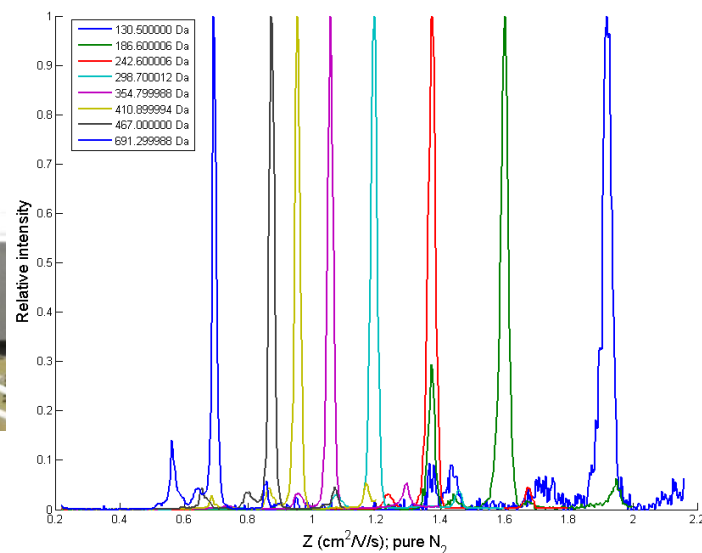
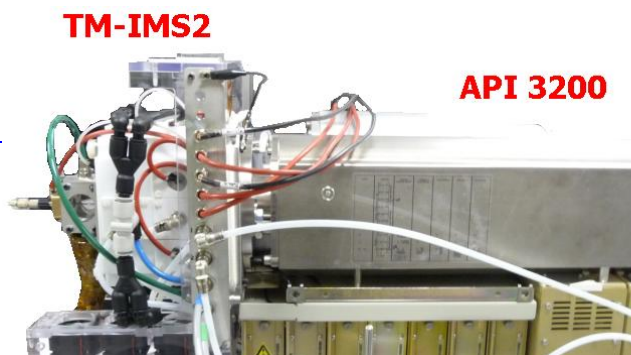
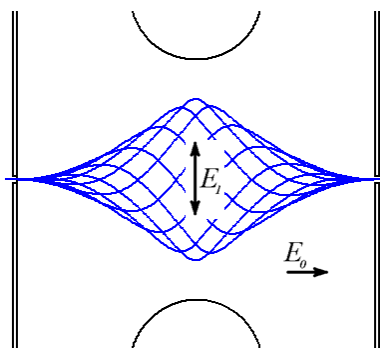


Transversal Modulation IMS. (TMIMS)

“Ion Mobility MS: New Instrumentation & Enabling Technologies”



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Summary

- Principle of operation:
- Demonstrator 1: TMIMS1:
 - Proof of concept: Resolving power & Robustness.
- Demonstrator 2: TMIMS2-MS:
 - Architecture.
 - IMS & IMS² modes.
 - Orthogonality.
- Numerical simulations.
- Conclusions.
- Challenges.

- Uniform electric fields:

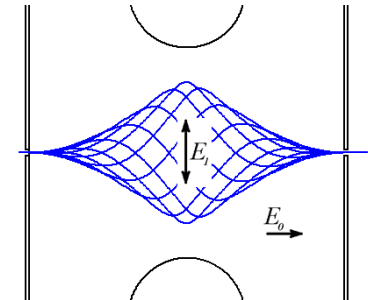
- Velocity \rightarrow trajectories:

$$u = KE_0$$

$$x = KE_0(t - t_0)$$

$$v = KE_1 \sin(\Omega t)$$

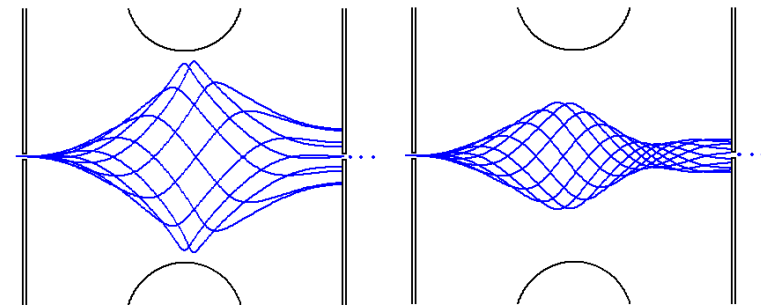
$$y = 2 \frac{KE_1}{\Omega} \sin\left(\frac{\Omega}{2}(t - t_0)\right) \sin\left(\frac{\Omega}{2}(t + t_0)\right)$$



- Distance to the outlet slit

$$Y = 2 \frac{KE_1}{\Omega} \sin\left(\frac{\Omega l}{2KE_0}\right) \sin\left(\Omega t - \frac{\Omega l}{2KE_0}\right)$$

\uparrow
 $= 0$

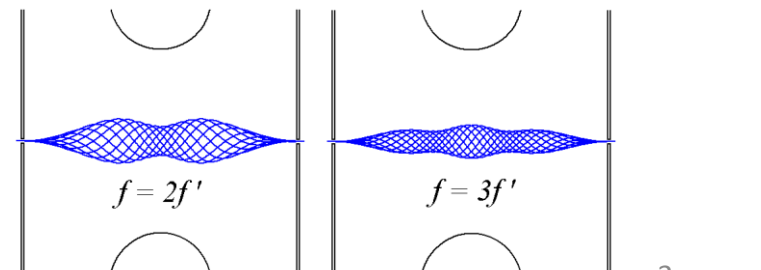


- Selection criterion:

$$K = \frac{\Omega l}{2\pi E_0}$$

- Higher resonances

$$K_n = \frac{\Omega l}{2n\pi E_0}$$



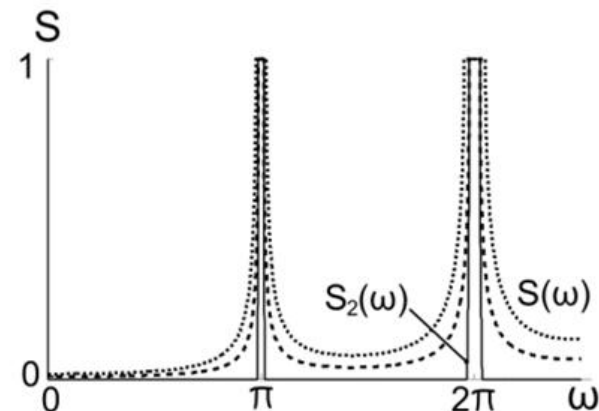
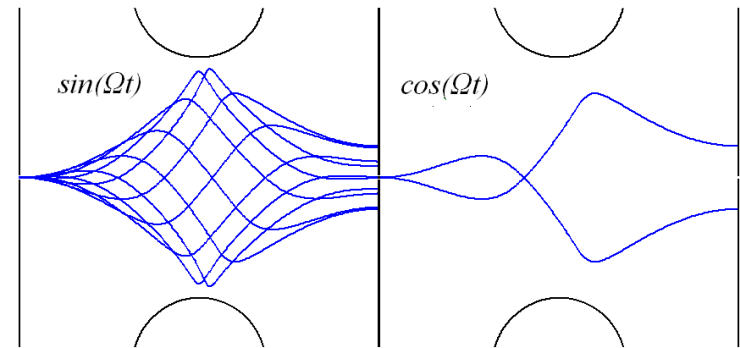
Two stages

- One stage produces a pulsed output:

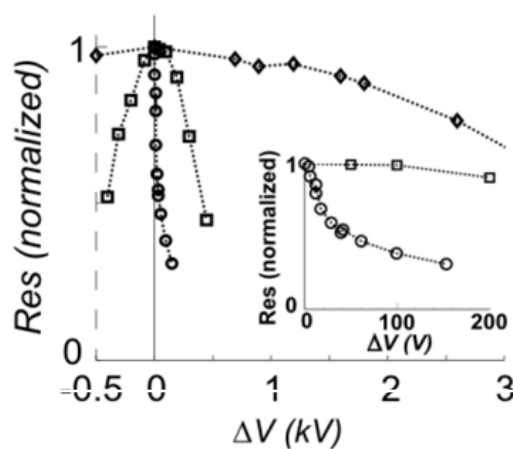
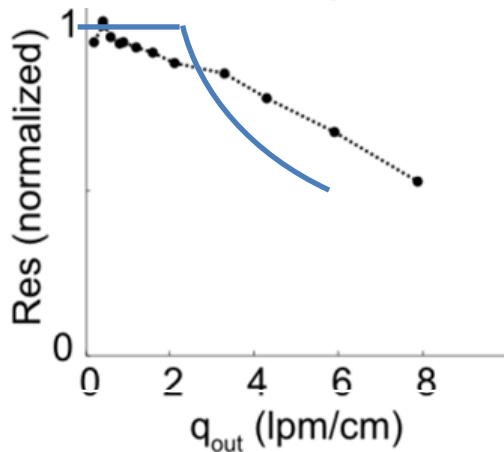
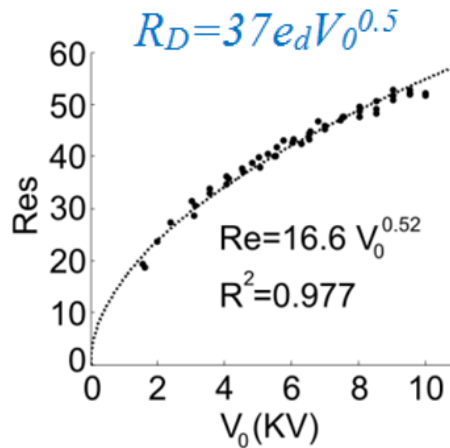
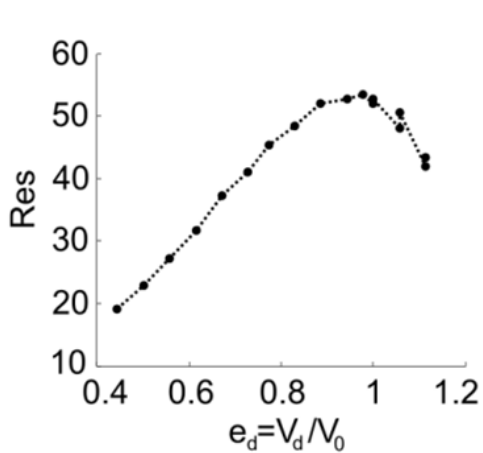
$$Y = 2 \frac{KE_1}{\Omega} \sin\left(\frac{\Omega l}{2KE_0}\right) \sin\left(\Omega t - \frac{\Omega l}{2KE_0}\right)$$

$\nearrow = 0$

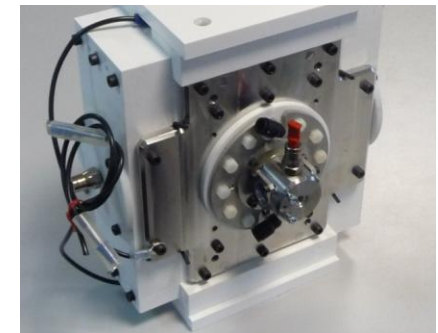
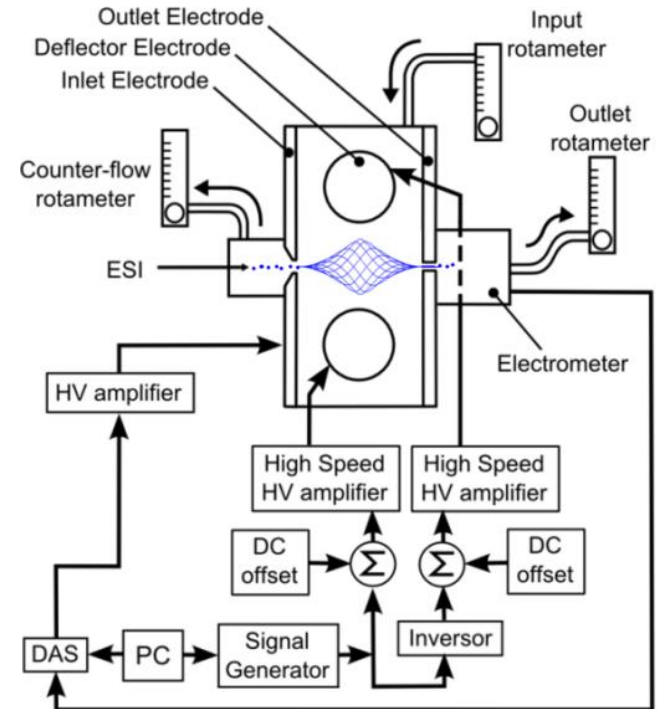
- Two stages operated in quadrature (same frequency) eliminate the pulsed output.
- Each stage can be operated with a different gas and a different voltage
 - IMS-IMS** analysis.



Resolving power & Robustness



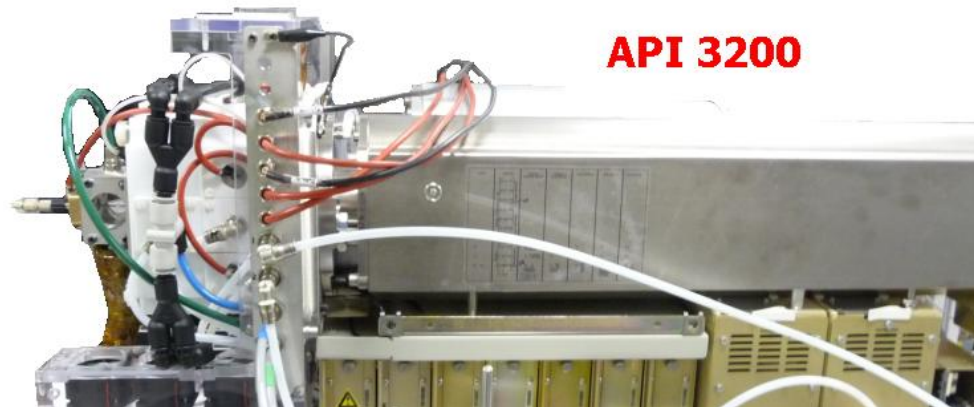
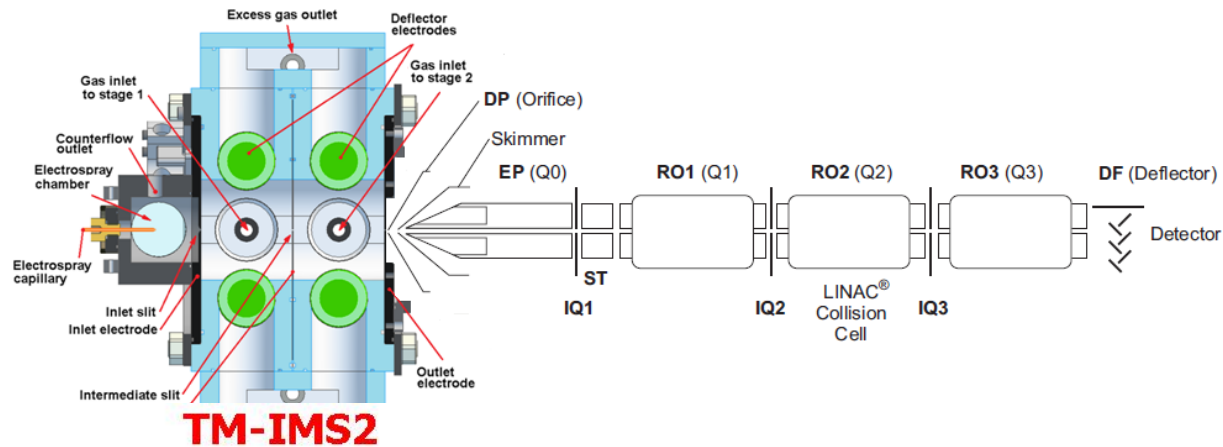
- One TMIMS stage; Nano-ESI; Electrometer.



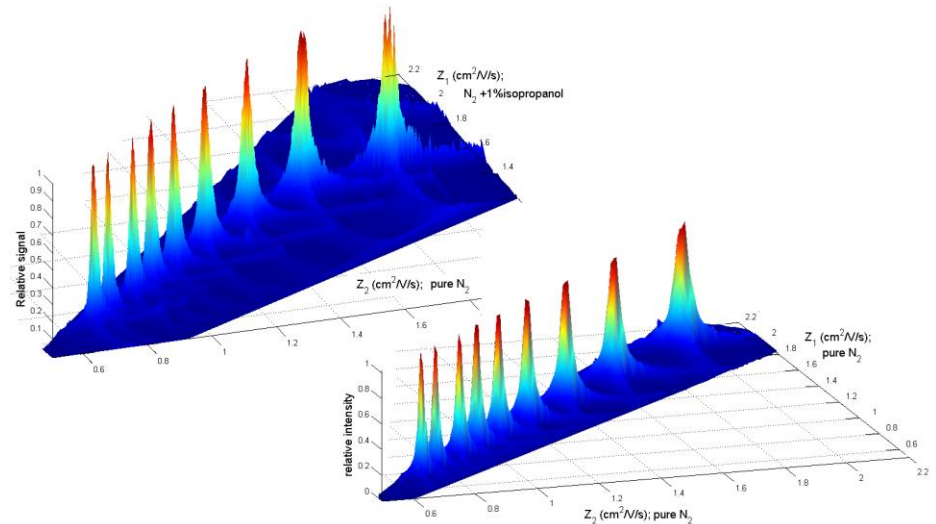
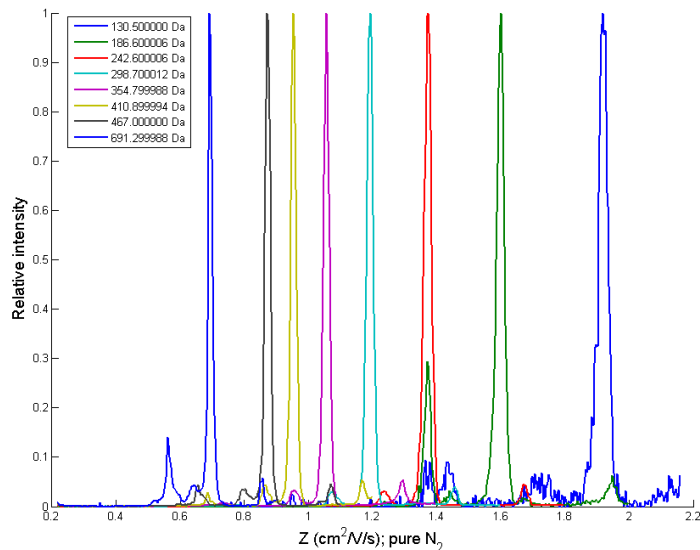
-Transversal voltage: circles; Longitudinal voltage: squares;
Different wave amplitude voltages: diamonds

TMIMS2-MS, Architecture.

- IMS-MS selection with a continuous output.
- TM-IMS² enhances peak capacity.



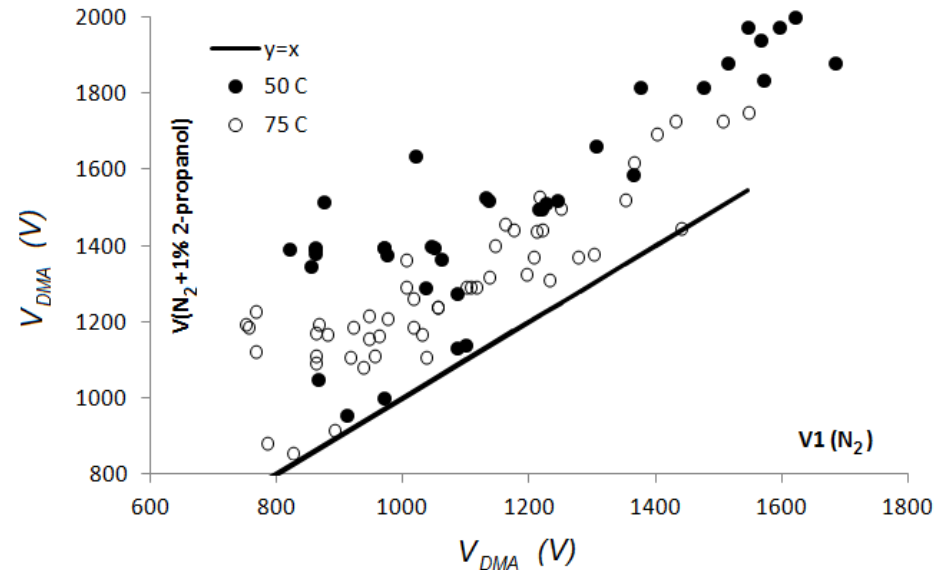
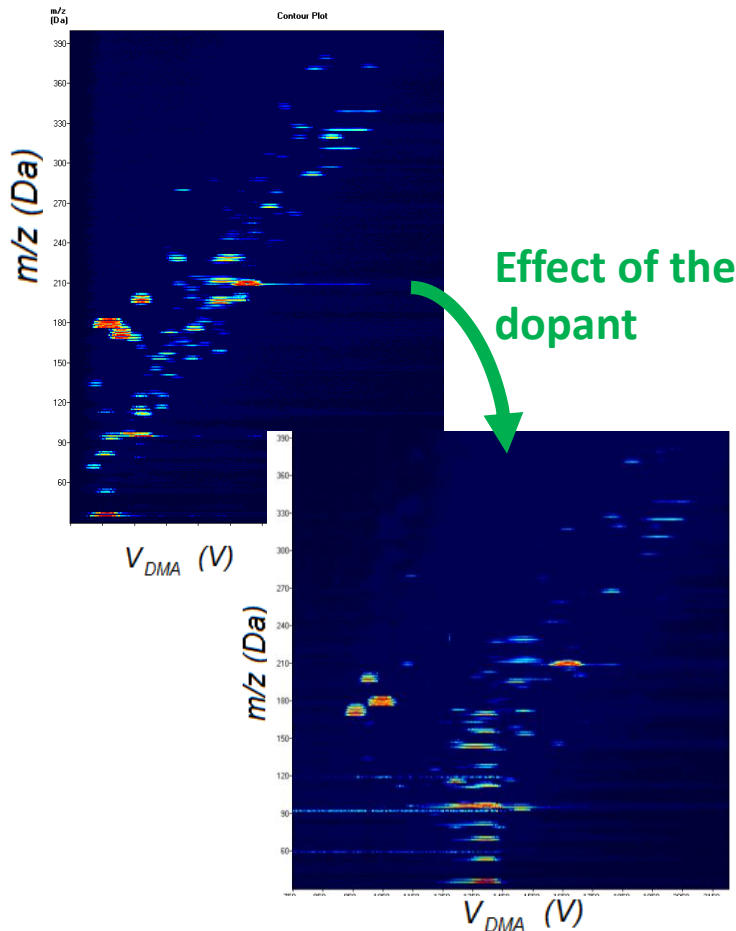
- Tetra alkyl ammonium ions. (Ethyl -Dodethyl).



- And transparent mode too.
 - Peak search strategies enable IMS² operation with moderate operational time.

IMS² Orthogonality

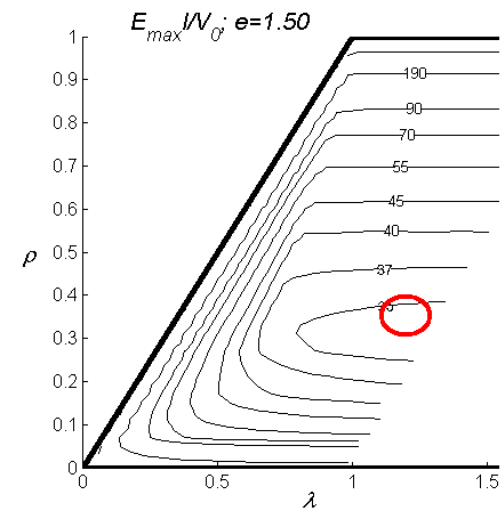
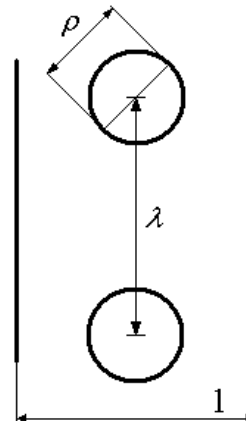
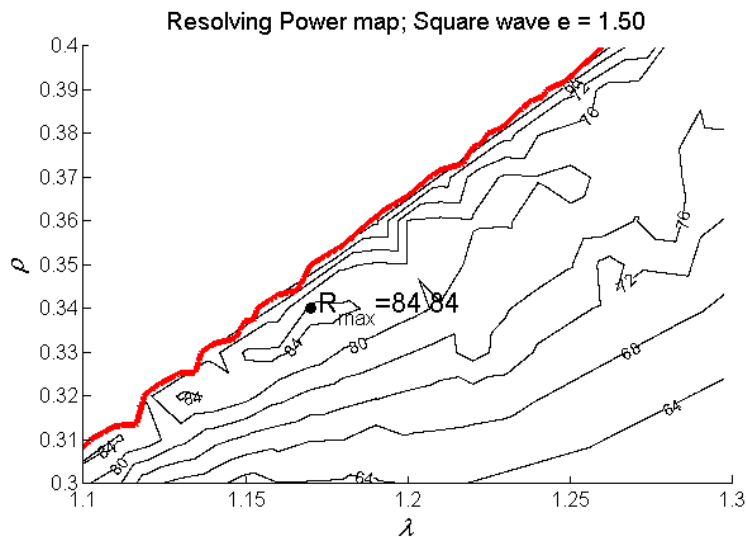
- Dry N₂ vs N₂ doped with 1% 2-propanol
- DMSO-Octanol-HCl nano-ESI; DMA-MS spectra.



- 2-propanol affects each species differently.
- It is a promising result, but orthogonality still needs to be characterized for the samples of interest.

Numerical simulations

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





Conclusions

- Current prototypes demonstrate:
 - IMS-IMS and IMS pre-filtration, with interesting IMS-IMS orthogonality.
 - Resolving power of 60 in IMS mode.
 - Resolving power of 40 in each stage IMS-IMS mode.
 - Estimated separation capacity: $40 \cdot (1 + 40 \cdot 20\%) = 360$.
 - Robustness, atmospheric pressure operation continuous output and :
 - facilitate coupling with most pre-existing MS.
- Numerical simulations show:
 - Optimized geometries would reach $R=80$.
 - Separation capacity would be $80 \cdot (1 + 80 \cdot 20\%) = 1360$

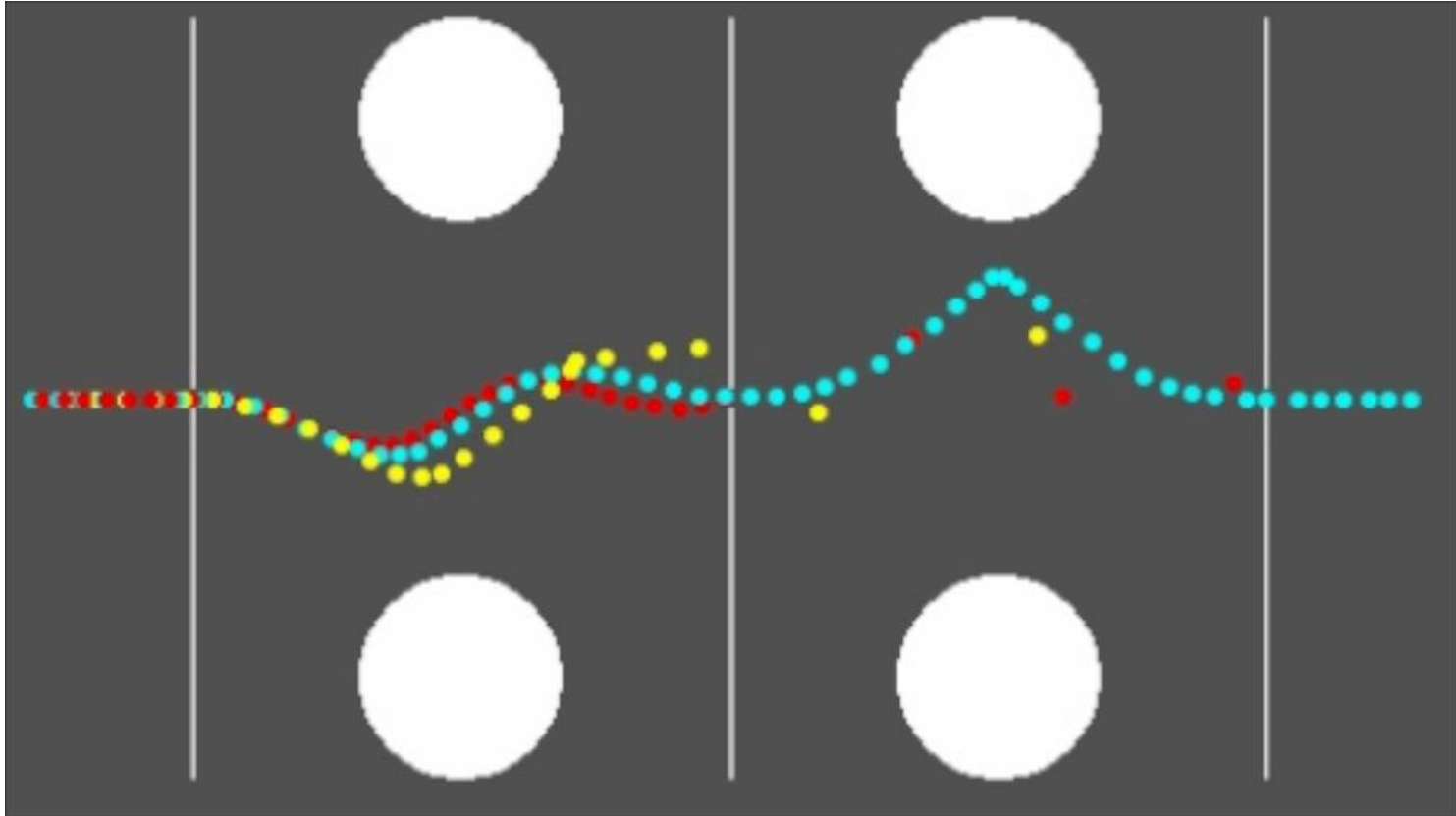


TMIMS Challenges

- Couple with commercial ion sources.
- Improve transmission.
- Reduce size and cost of the High Voltage system.
- ...
- **Bring the tool to life by using it!**



Thanks for your attention!



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