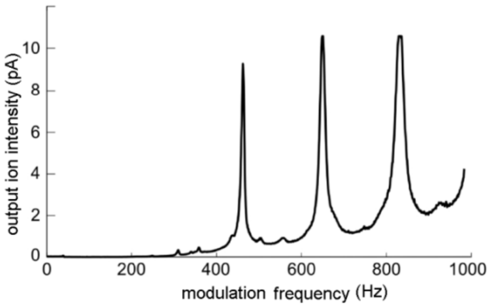
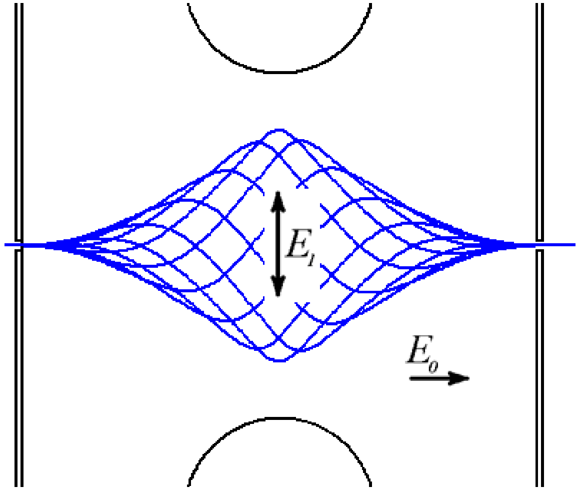
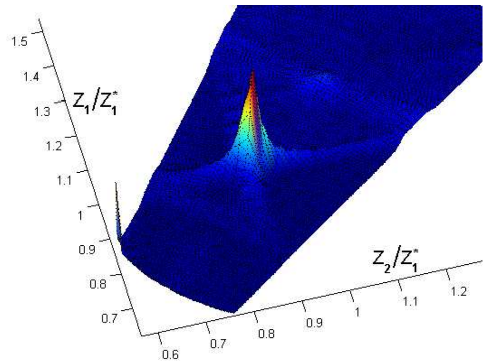
Transversal Modulation IMS. (TM-IMS)

"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.

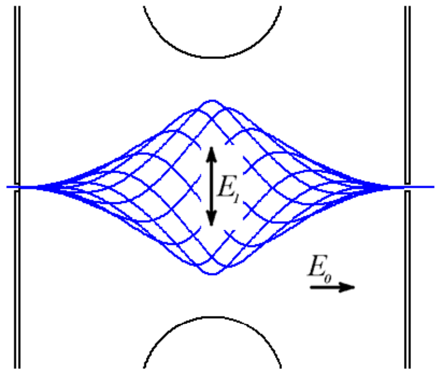
- Ideal uniform electric fields:
  - Velocity → trajectories:

$u = KE_0$

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

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

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



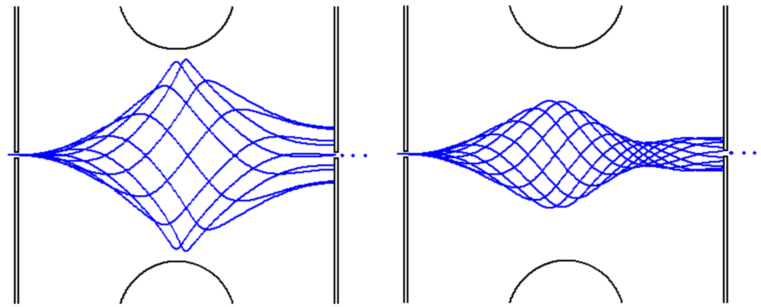
  - Distance to the outlet slit

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

$= 0$

  - Selection criterion:

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

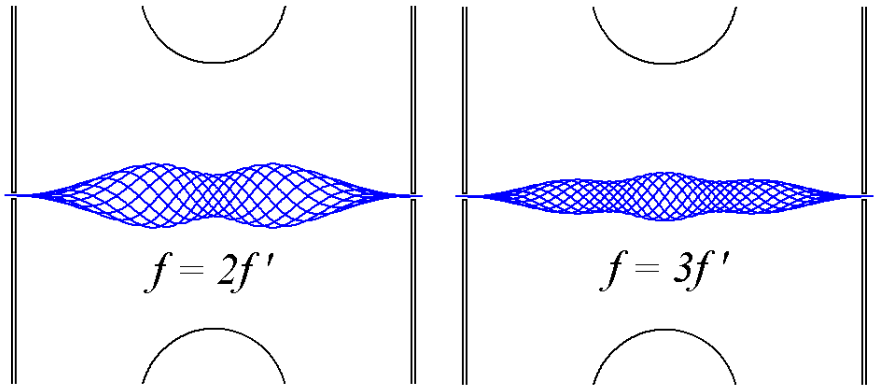


Principle of operation: Higher resonances.

- 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 $K_2 = K_1/2$.



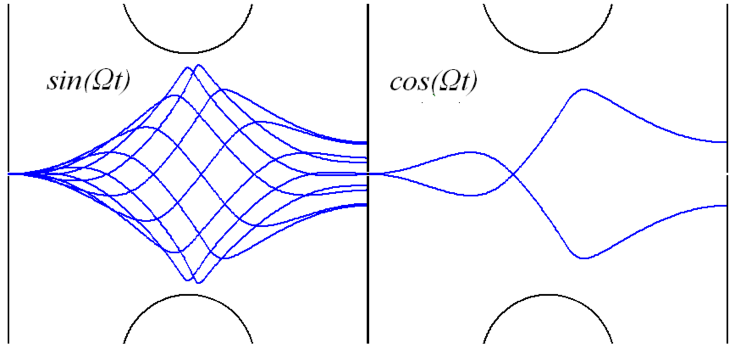
Principle of operation: Two stages.

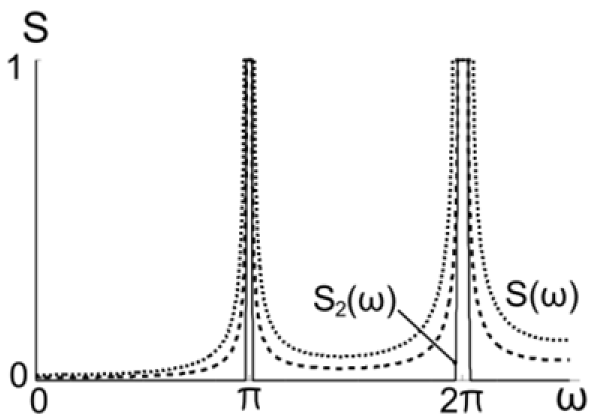
- One stage produces a pulsed output of non desired ions:

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

$= 0$

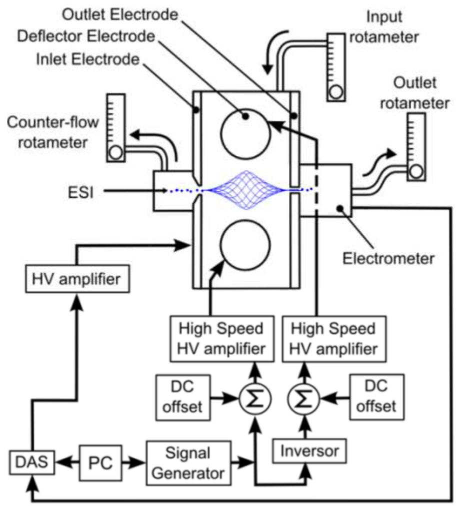
- Two stages operated in quadrature (same frequency) eliminate the pulsed output.
- Each stage can be operated with a different gas and a different voltage
  - ***IMS-IMS** analysis.*





TMIMS-1: Architecture.

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



Anal. Chem., 2012, 84 (18), pp 7831–7837

TMIMS-1: Resolving power (*Res*).

Theoretical estimation

- Ions spread due to diffusion.

$$\sigma^2_r = 2D\tau$$

- Calculate instantaneous signal $N(Y, \sigma_r)$

$$S = \frac{1}{\sqrt{2\pi}\sigma_r} e^{-\frac{\left(\frac{E_1}{E_0}\frac{K-K_0}{K_0}\sin(\Omega t)\right)^2}{2\sigma_k^2}}$$

- Integrated averaged signal.

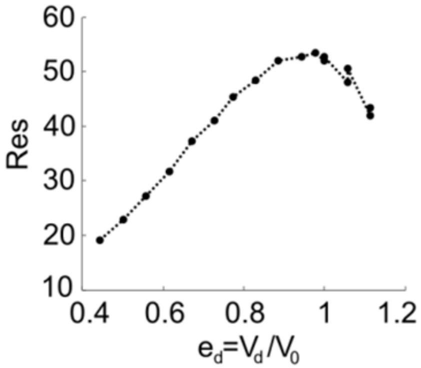
$$\overline{S} = \int_0^{2\pi} e^{-\frac{1}{2}\left(K/K_0 - 1\right)^2 A\cdot\sin^2(\theta)} d\theta$$

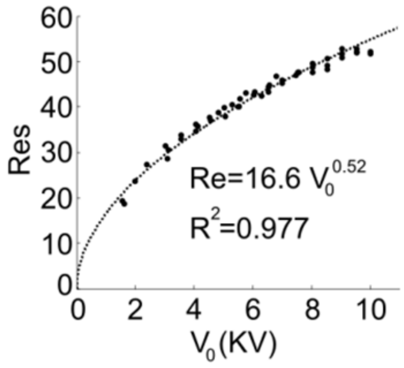
- Reconstruct spectrum, FWHH.

$$R_D \approx 0.187 \frac{E_1}{E_0}\sqrt{\frac{V_0 e}{k_B T}}$$

Experimental results

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





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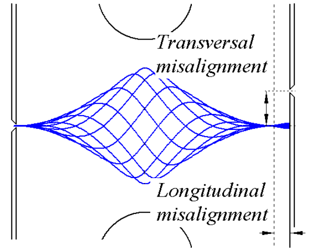
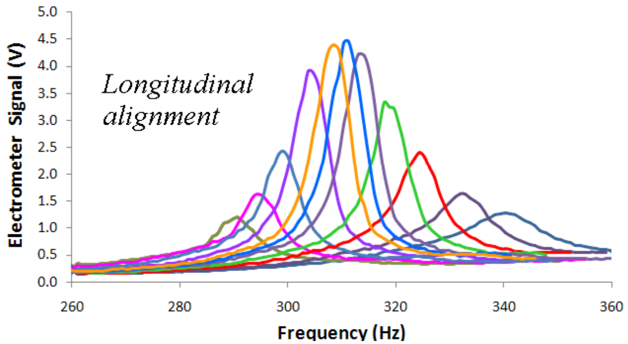
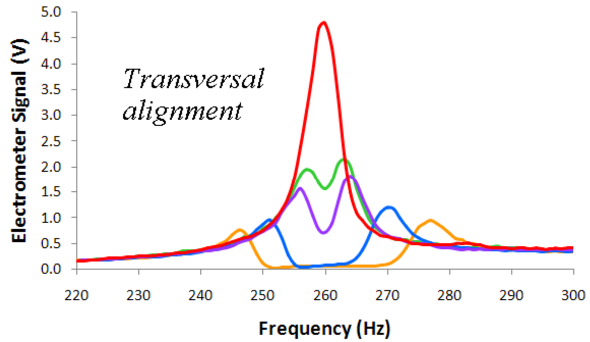
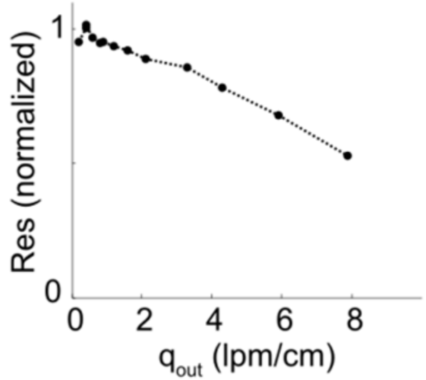
TMIMS-1: Robustness.

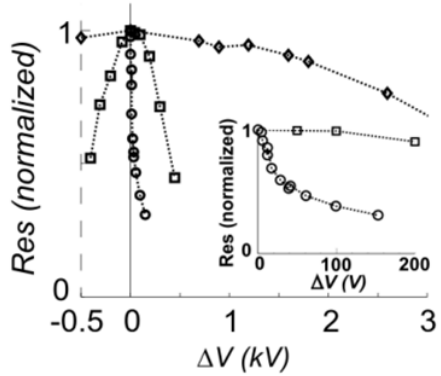
- Electronic alignment compensates for mechanical misalignments.
  - Tolerates mechanical misalignments as high as 1mm.
  - Tolerates 5V error in mean deflector voltage.







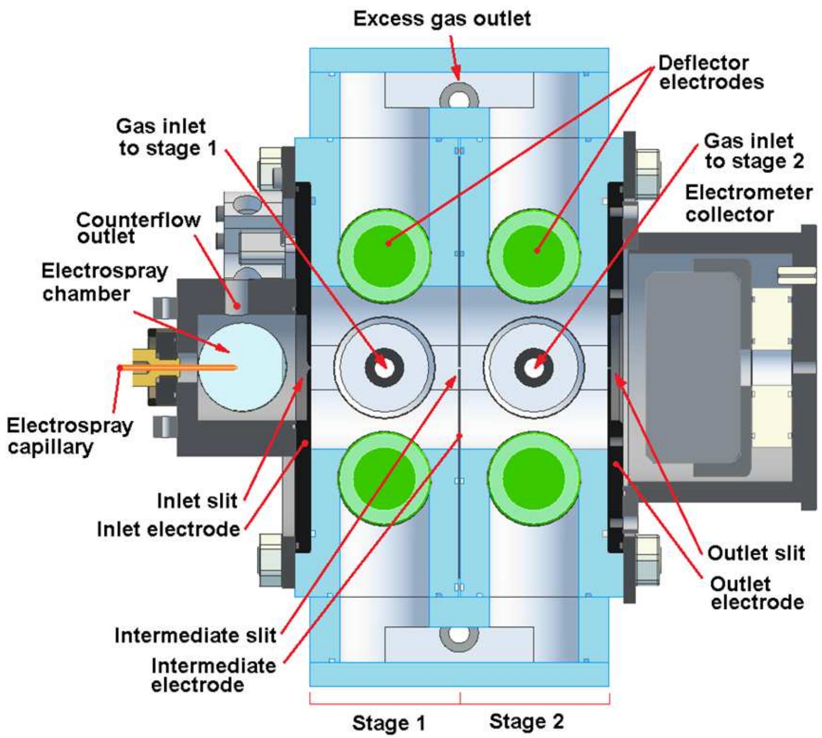




-Transversal voltage: circles
-Longitudinal voltage: squares
- Different wave amplitude voltages: diamonds

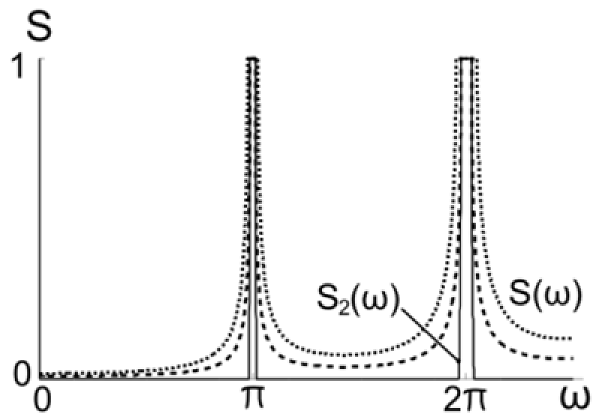
TMIMS-2: Architecture.

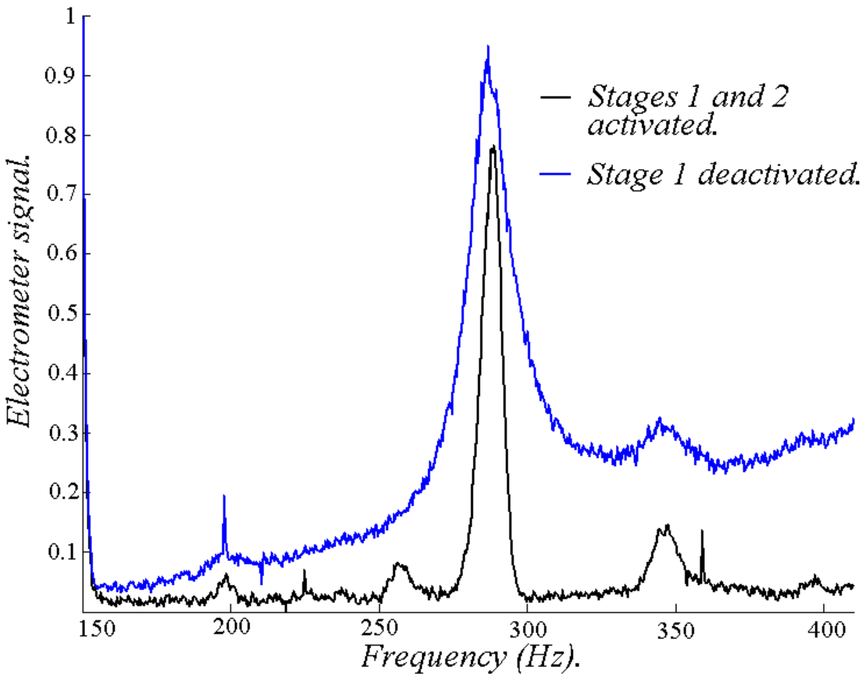
- Two stages.
- Two gases.
- Nano-ESI ion source
- Electrometer detector
- IMS and IMS^2 analysis



TMIMS-2: Background reduction.

- Synchronization of Stages eliminates pulsed signals

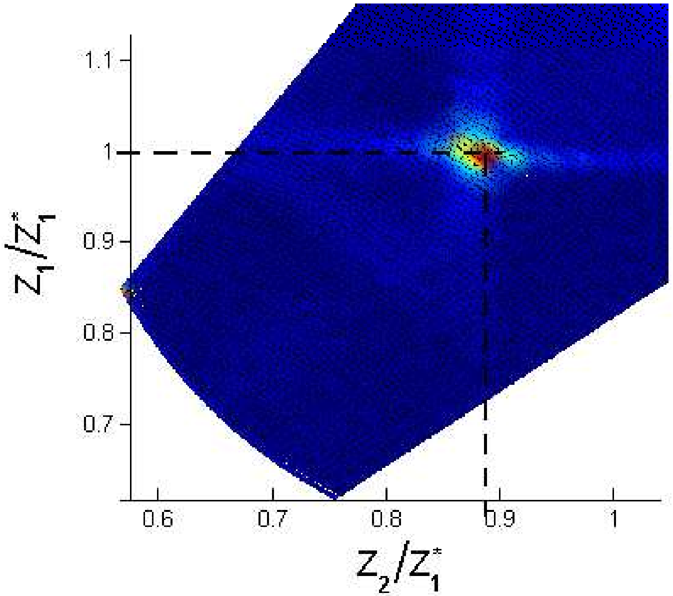


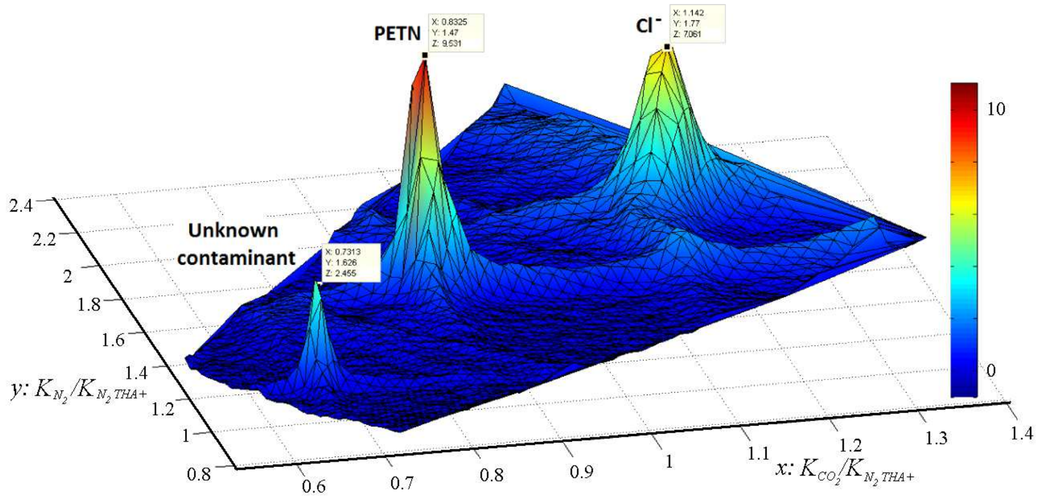


TMIMS-2: IMS^2

- ESI: MeOH, H2O, THABr.
- Stage 1: N_2
- Stage 2: N_2 with 1% iso-propanol.

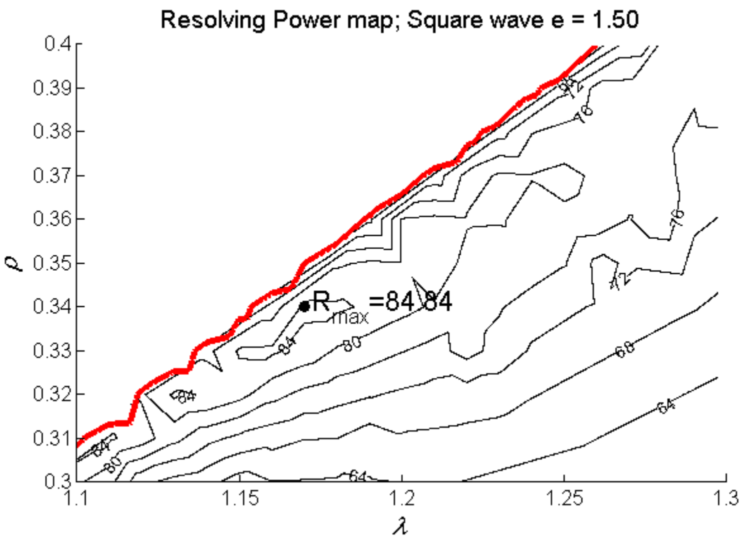
- ESI: MeOH, H2O, HCl, PETN
- Stage 1: CO_2
- Stage 2: N_2

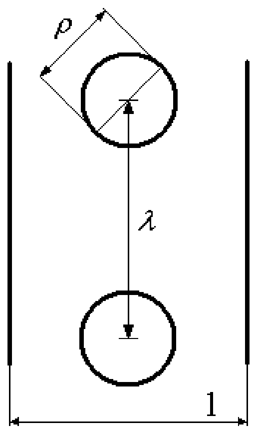


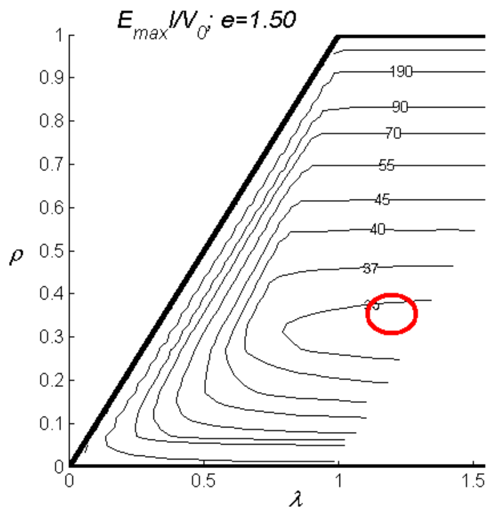


Numerical simulations:

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







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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.

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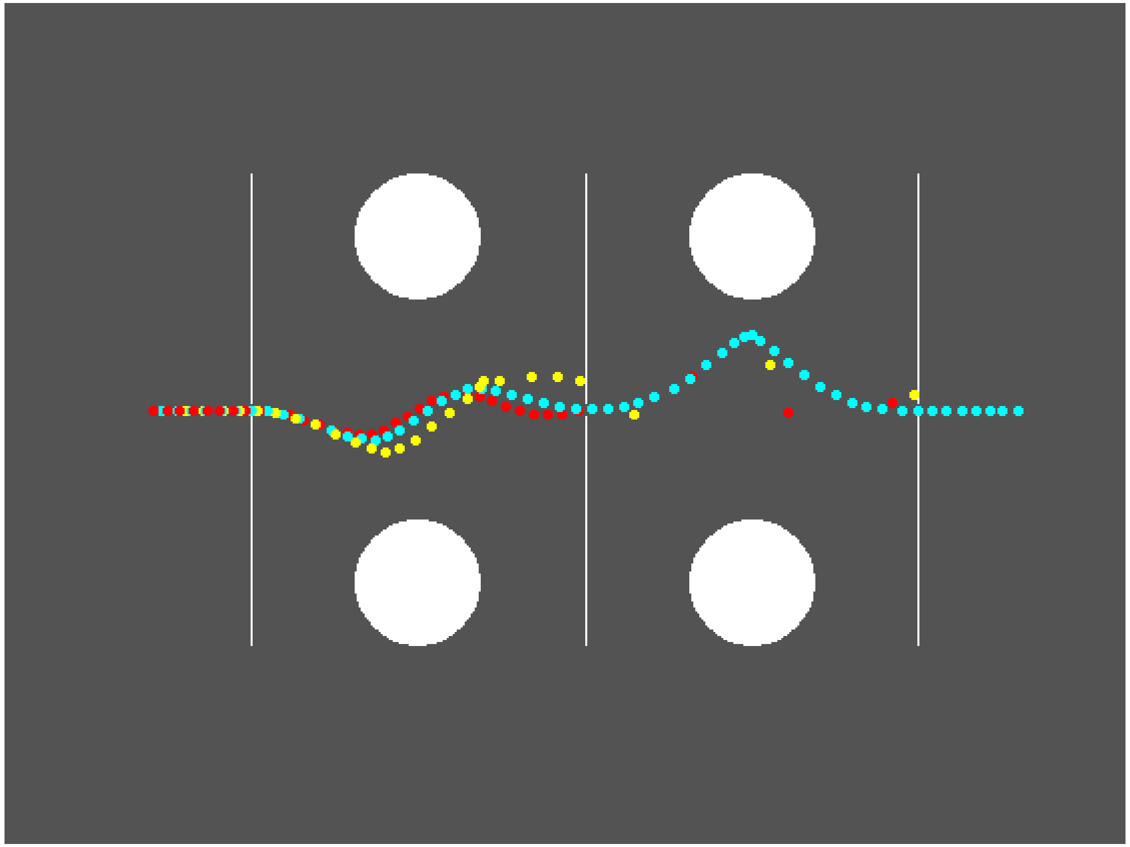
Thanks for your attention!



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