New planar DMA designs for high transmission and resolution coupling to modern API-MS instruments

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Spanish R&D micro-business established in February 2005

Objective: developing a new technology for explosives detection

Since 2005, SEADM has completed or is currently developing the following projects:

- **EXPLOSIVE TRACE DETECTION**
  - Demonstrator built detecting vapour traces of explosives in the atmosphere at concentrations of 1 ppt
  - Prototype development since January 2007: DETEV project. Explosive trace detector unit to be used in road control.

- **DMA-MS INTEGRATION**
  - MAIMS Program (Mobility Analysis Integrated with Mass Spectrometry), since September 2006, to couple a DMA (Differential Mobility Analyzer) to an API Mass Spectrometer, in order to increase its resolution capability for biological analysis. MAIMS is an international Canadeka program and is partially funded by the Spanish Ministry of Industry within the 2004-2007 I+D+i National Plan.

Located in Boecillo (Valladolid), 250 m² laboratory. Staff of 6 engineers
Mobility separation in a planar DMA

Inlet slit of charged particles of several mobilities

Uniform flow at velocity $U$

Electric Field $E = \frac{V_{DMA}}{\Delta}$

Exit hole of particles at mobility $Z = \frac{U\Delta^2}{LV_{DMA}}$

$\Delta$

$L$
Mechanical design of the planar DMA
Planar DMA performance – Diffusion

\[ FWHH^2 = 16 \ln 2 \left( \frac{L}{A} + \frac{A}{L} \right) (1/Pe) \]

\[ Pe = Re \frac{v}{D} \]

FWHH < 1 % requires Reynolds ~ 40,000 for ions of 1 cm²/Vs

The aerodynamical design has been operated under laminar conditions up to Reynolds = 200,000
Planar DMA performance – $q_{out}$

2-D sampling across the chamber $\Rightarrow$ $FWHH = \frac{q_{out}}{Q} \Rightarrow FWHH < 0.1 \%$

$FWHH \approx (kq_{out}/Q)^{1/2}(1 + \Delta^2/L^2)^{1/4}$

Typical values:
$q_{out} = 0.5$ lpm
$Q = 1000$ lpm
$FWHH \sim 3 \%$
Resolving power $\sim 30$
Prototypes progression – P1

First prototype (P1):
- Not to be coupled to any other instrument
- Many different configurations tested, for theories comparison and models adjustment
- Barely below 2 % resolution (Resolving power < 50)
Prototypes progression – P2

Second prototype (P2):
- Coupled to API 365 and API 3000 triple quads
- $q_{out} = 0.3 - 0.5$ lpm
- Resolving power > 50
- Currently at MDS Sciex, Toronto → published results of >5x sensitivity improvement (ASMS 08)

Tetraethylammonium$^+$ ($\sim 1.8 \text{ cm}^2/\text{Vs}$)
Prototypes progression – P3 (1/2)

Third series of prototypes (P3)
- Coupled to API 365 triple quad and to QStar QqTOF
- Similar to P2 in aerodynamic design and operation
- Mechanical redesign, higher operating voltages
A planar DMA coupled to a MS for tandem IMS-MS separation at high transmission, with IMS resolution approaching 100. Rus J.; Estevez F.; Fernandez de la Mora J.; Proc. 57th ASMS Conf. Mass Spectrom. All. Top.; Indianapolis (Indiana) USA June, 2007
Fourth series of prototypes (P4):
- Coupled to API 365 triple quad and to QStar QqTOF
- $q_{out} = 0.5 \text{ lpm}$
- Resolving power > 50
- Improved transmission through outlet
- Optimized for larger (less mobile) analytes

Coulombic denaturing of gas phase proteins electrosprayed from neutral aqueous solutions studied by IMS (DMA) MS; Fernandez de la Mora J.; Proc. 58th ASMS Conf. Mass Spectrom. All. Top.; Denver (Colorado) USA June, 2008
Latest developments and future work

Higher flow rates sampled ($q_{out}$) and delivered to the MS

**Measuring DMA → MS transmission**

**Tandem DMA-DMA system developed by P. McMurry (U. Minnesota)**

**Coupling to modern API instruments, which sample higher flow rates:**
- Shimadzu’s LCMS2010EV single quad: 1.0 lpm
- API 5000 triple quad: 2.9 lpm
Transmission measurements (1/2)

Delivers a flow of monomobile ions at a concentration $n_{in}$ to be sampled by the second DMA (the one tested for transmission).

Transmission = $I_{out}/I_{max}$

$I_{max}$ = Maximum signal through the DMA: $q_{out} \cdot n_{in}$

$n_{in} = I_{aux} / q_{aux}$
Transmission measurements (2/2)

- DMA at M~0.17, THA+ peak at 2000 V
- DMA at M~0.10, THA+ peak at 1250 V

Flows per unit length. 3D effects at the outlet not considered.

- Auxiliary DMA
- Tested DMA
- 2 way valve
- Auxiliary electrometer

Graph: Scatter plot showing transmission (%) vs. $q_i / q_{out}$ (%) with red and black dots indicating different DMA conditions. The graph notes flows per unit length and 3D effects at the outlet not considered.
Higher $q_{out}$ delivered to the MS (1/2)

- Modified P3 instrument
- Delivers ions to a capillary MS inlet (instead of chocked orifice)
- Highest resolving powers achieved (> 100) even with the doubled $q_{out}$

![Graph showing resolution improvement by decreasing inlet flow of ions](image)

![Graph showing DMA voltage vs. sample flow](image)
Higher $q_{out}$ delivered to the MS (2/2)

- Already coupled to Shimadzu’s LCMS 2010 EV single quad

<table>
<thead>
<tr>
<th>THA$^+$ peak voltage (V)</th>
<th>Mach number</th>
<th>Resolving power</th>
<th>FWHH</th>
<th>$s$</th>
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<tbody>
<tr>
<td>3900</td>
<td>0.23</td>
<td>65</td>
<td>1.50%</td>
<td>0.13%</td>
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<tr>
<td>5300</td>
<td>0.31</td>
<td>80</td>
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<td>0.09%</td>
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<tr>
<td>6500</td>
<td>0.40</td>
<td>86</td>
<td>1.16%</td>
<td>0.09%</td>
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</tbody>
</table>

THABr 100 µM
Conclusions

- Series of planar DMA prototypes designed and manufactured with resolving powers exceeding 50, approaching 100
- Different designs have been coupled to Sciex’s API 365, API 3000, QStar and Shimadzu’s LCMS2010EV
- Full transmission of ions from the inlet to the outlet. Transmission limited by achievable inlet flow: inserted up to 50% of MS flow rate $\rightarrow$ 50 % DMA-MS transmission
- New designs tackle the $q_{out}/Q$ limitation approaching the target $q_{out} = 3$ lpm while keeping resolving power 50-100
Acknowledgments – SEADM DMA team

And thank you!