An Evaluation of a Particle Beam Interface at High Aqueous Concentrations

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Problem...

Reverse phase HPLC can typically include high aqueous solvent conditions.

MS is becoming a preferred detection device for HPLC.

Compatibility between the two techniques is challenging.
Stages of Particle Beam LC/MS

HPLC

INTERFACE

MASS DETECTOR

LC Liquid Phase

Phase Separate

Momentum Separate

MS Gas Phase
INTERFACE

Phase Separate
Aerosol generation
Desolvation

Momentum Separate
Enrichment/Pressure Reduction
Phase Separation

- Goal
  To separate the solvent from the solute by converting the solvent to the gas phase and the solute to particles
  - Nebulization - generation of an aerosol
  - Desolvation - separation of the solvent from the solute
Momentum Separation

Goal
To remove gas phase while transporting particles into MS
- Effective removal of solvent
- Enrichment of solute
INTERFACE

Phase Separate

Aerosol generation
Desolvation

Momentum Separate

Enrichment/Pressure Reduction
Phase Separation

Why are some solvent conditions more difficult?
## Phase Separation

<table>
<thead>
<tr>
<th>Solvent</th>
<th>B.Pt.</th>
<th>Hvap</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Protic</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>100</td>
<td>10.5</td>
</tr>
<tr>
<td>Methanol</td>
<td>64.7</td>
<td>8.9</td>
</tr>
<tr>
<td><strong>Aprotic</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acetonitrile</td>
<td>81.6</td>
<td>7.8</td>
</tr>
<tr>
<td>THF</td>
<td>66.0</td>
<td>7.6</td>
</tr>
</tbody>
</table>
Phase Separation

\[ (C_{pdtx})_{l} + (C_{pdtx})_{g} \rightarrow (C_{pdtx})_{sol} \]

\[ \Delta H_{vap} \]

TOC measured

Power (watts)

100% Solvent Evaporation
0% Solute Evaporation
Summary of Phase Separation

ThermaBeam™

Thermal/Pneumatic Nebulization Desolvation
Analysis of Environmental Compounds

Experimental Conditions

Analytical Conditions

Compounds: caffeine
methomyl
benzidine

Column: Waters Nova-Pak C18 (2.0 x 150 mm)

Mobile Phases: (1) 72:28 ammonium acetate:ACN
(2) 87:13 ammonium acetate:ACN

Flow rate: 250 μL/min
MS Review

Solvent Conditions
72:28
NH$_4$OAc:ACN
Maxplot Chromatogram

100 to 200 amu
High Aqueous Solvent Conditions
87:13
NH OAc:ACN 4
MS Review

High Aqueous Solvent Conditions
87:13
$\text{NH}_4\text{OAc:ACN}$
View Cube

3D Chromatogram
Mass Spec Review: Extraction

TIC
Contour View

Maxplot
Chromatogram
Maxplot Chromatogram
100 to 200 amu
Overlay of Mass Spectra

Spectrum Review

File Edit Plot Derived Library Help

Counts

20000.0

6000 8000 10000 12000 14000 16000 18000 20000

AMU

# 1 Extracted Base Peak 109 AMU 3.321 minutes 16957 Counts 50 - 200 AMU

# 2 Extracted Base Peak 57 AMU 4.294 minutes 7083 Counts 50 - 200 AMU

# 3 Extracted Base Peak 184 AMU 18.748 minutes 35571 Counts 50 - 200 AMU
Extracted Mass Spectrum of methomyl
Extract a Mass Spectrum of benzidine
Extracted Mass Spectrum of benzidine
Extract a Mass Spectrum of caffeine
Extracted Mass Spectrum of caffeine
Conclusions

- Analysis using high aqueous solvent conditions is possible
- ThermaBeam™ lessens the challenge for compatibility between HPLC and MS
- AutoOptimize adjusts the interface to handle high aqueous conditions