Evaluation of Small Mass Spectrometer Systems

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Introduction

Understand Aspects of Designing a Miniature Mass Spectrometer (MS) System

Systems Evaluated
- Linear Quadrupole
- Quadrupole Ion Trap
- Sector
- Quadrupole Array
- Time of Flight

Figures of Merit
- Accuracy
- Limits of Detection
- Response Time
- Volume
- Precision
- Scan Rate
- Recovery Time
- Weight

Set Up Scale to Rank Systems
Why Miniaturize?

• **Improve Portability**
  - Field Applications
  - Real-Time Analysis
  - Decrease Contamination

• **Size Reduction**
  - Increase Sensor Density
  - Less Intrusive

• **Cost Reduction**
  - Less Weight
  - Less Power
Potential Applications

- **Leak Detection**
  - Hazardous Gases
  - Helium
  - Refrigerants

- **Air Analysis**
  - Worker Safety
  - Public Safety
  - Chemical Weapons

- **Law Enforcement**
  - Contraband Detection

- **Field Medical Analysis**

- **Process Control**
  - Semiconductors
  - Hydrogen Economy
NASA Applications

- Next-Generation Leak Detection During
  Processing
  Cryogenic Fueling
  Launch Countdown

- Shuttle Engine Monitoring

- Air Analysis
  International Space Station Air Lock
  Shuttle Air Lock

- Process Control
  Martian Fuel Generators
Current Problems

Response Time  |  Scan Rate  |  Sampling Density
Stanford Research Systems (SRS) RGA-100

• Linear Quadrupole Analyzer
  Cylindrical Rods: 6.35mm OD
  Rod Length: 11.4 cm
  Inscribed Radius: 2.77 mm
  Frequency: 2.76 MHz

• Pressure = $5 \times 10^{-5}$ torr

Inficon XPR-2

• Linear Quadrupole Analyzer
  Hyperbolic Rods
  Rod Length: 12.7 mm
  Inscribed Radius: 0.33 mm
  Frequency: 13 MHz

• Pressure = $1 \times 10^{-4}$ torr
**Ferran**

- Quadrupole Array System
  - 16 Cylindrical Rods: 1 mm OD
  - Rod Length: 10 mm
  - Frequency = 16 MHz
- Pressure: $5 \times 10^{-4}$ torr

**IonWerks Time-of-Flight (TOF)**

- Reflectron TOF System
  - Orthogonal Acceleration
  - Extraction Pulse: 600 V
  - Sampling Rate: 50 kHz
- Pressure: $5 \times 10^{-6}$ torr
University of Florida Ion Trap (UF-IT)

- Quadrupole Ion Trap System
  Ring Radius: 10 mm
  Stretched Geometry
  Frequency = 2.5 MHz
  No Buffer Gas
- Pressure: $4 \times 10^{-6}$ torr

Thermo Finnigan Polaris-Q

- Quadrupole Ion Trap System
  Ring Radius: 7 mm
  Stretched Geometry
  Frequency = 1.03 MHz
  Helium Buffer Gas
- Pressure: $1 \times 10^{-3} (4 \times 10^{-6})$ torr
Monitor Group
MG-2100

• Cycloidal Sector System
  B: 0.5 tesla
  Pitch: 1 inch

• Pressure: $5 \times 10^{-6}$ torr

University of Minnesota
Compact Double Focus MS (CDFMS)

• Double Focus Sector System
  B: 0.75 tesla
  Sector Radius: 20 mm

• Pressure: $10^{-5}$ torr
## Experimental Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Shuttle Requirement</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Accuracy</strong></td>
<td>$\frac{\bar{\gamma}<em>{\text{test, meas}}}{\bar{\gamma}</em>{\text{true}}} \times 100%$</td>
<td>&lt; 10% or 5 ppm, whichever is greater</td>
</tr>
<tr>
<td><strong>Precision</strong></td>
<td>$\frac{\bar{\gamma}<em>{\text{test, meas}}}{\bar{\gamma}</em>{\text{true}}} \times 100%$</td>
<td>&lt; 5% or 3 ppm, whichever is greater</td>
</tr>
<tr>
<td><strong>Limit of Detection</strong></td>
<td>$3 \times \text{zero}^a$</td>
<td>$\text{H}_2, \text{O}_2$: 25 ppm; He: 100 ppm; Ar: 10 ppm$^b$</td>
</tr>
<tr>
<td><strong>Response Time</strong></td>
<td>Time required for response from valve change to 95% new reading</td>
<td>10 s</td>
</tr>
<tr>
<td><strong>Recovery Time</strong></td>
<td>Time after valve change to reach 5% of previous sample reading (new sample is zero)</td>
<td>30 s</td>
</tr>
<tr>
<td><strong>Scan Rate</strong></td>
<td>Experiment time / scans</td>
<td>1 s</td>
</tr>
<tr>
<td><strong>System Volume</strong></td>
<td>Sum of individual components</td>
<td>$3.5 \times 10^4 \text{ cm}^3$</td>
</tr>
<tr>
<td><strong>System Weight</strong></td>
<td>Sum of individual components</td>
<td>10 kg</td>
</tr>
</tbody>
</table>

$^a$ Theoretical limit of detection  
$^b$ Measured limit of detection
Experimental Scan

Response (Arbitrary)

Time (min.)

0 5 10 15 20 25

Span

Test

Zero

Test

Zero
Accuracy

Accuracy (Absolute Value) (%)

Hydrogen
Helium
Oxygen
Argon

SRS  XPR-2  Ferran  Polaris-Q  UF-IT  TOF  MG-2100  CDFMS
Limits of Detection (LOD)

- Hydrogen
- Helium
- Oxygen
- Argon

 LOD (ppm)

- SRS
- XPR-2
- Ferran
- Polaris-Q
- UF-IT
- TOF
- MG-2100
- CDFMS

- Helium
- H₂ & O₂
- Argon

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Response Time

- SRS
- XPR-2
- Ferran
- Polaris-Q
- UF-IT
- TOF
- MG-2100
- CDFMS

Response Time (s)

- Hydrogen
- Helium
- Oxygen
- Argon

Values:
- SRS: 120, 130
- XPR-2: 130
- Ferran: 150
- Polaris-Q: 130
- UF-IT: 130
- TOF: 210
- MG-2100: 180
- CDFMS: 130

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Recovery Time

![Recovery Time Graph]

- Hydrogen
- Helium
- Oxygen
- Argon
Scan Time

Scan Time (s)

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Scan Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRS</td>
<td>6</td>
</tr>
<tr>
<td>XPR-2</td>
<td>1.8</td>
</tr>
<tr>
<td>Ferran</td>
<td>7.5</td>
</tr>
<tr>
<td>Polaris-Q</td>
<td>1</td>
</tr>
<tr>
<td>UF-IT</td>
<td>1</td>
</tr>
<tr>
<td>TOF</td>
<td>1</td>
</tr>
<tr>
<td>MG-2100</td>
<td>13</td>
</tr>
<tr>
<td>CDFMS</td>
<td>1</td>
</tr>
</tbody>
</table>
System Volume

![System Volume Graph]

- **Analyzer and Vacuum System**
- **Electronics**
- **Turbo Pump**
- **Rough Pump**

**Volume (cm^3)**

- SRS
- XPR-2
- Ferran
- Polaris-Q
- UF-IT
- TOF
- MG-2100
- CDFMS
System Weight

<table>
<thead>
<tr>
<th>SRS</th>
<th>XPR-2</th>
<th>Ferran</th>
<th>Polaris-Q</th>
<th>UF-IT</th>
<th>TOF</th>
<th>MG-2100</th>
<th>CDFMS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>50</td>
<td>40</td>
<td>50</td>
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<td></td>
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</table>

Legend:
- **Analyzer / Vacuum / Frame**
- **Electronics**
- **Turbo Pump**
- **Rough Pump**
## Evaluation Chart

<table>
<thead>
<tr>
<th></th>
<th>Accuracy</th>
<th>Precision</th>
<th>LOD</th>
<th>Response</th>
<th>Recovery</th>
<th>Scan Rate</th>
<th>System Volume</th>
<th>System Weight</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRS</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>6</td>
<td>8</td>
<td>6</td>
<td>7</td>
<td>4.3</td>
</tr>
<tr>
<td>XPR-2</td>
<td>3</td>
<td>8</td>
<td>2</td>
<td>7</td>
<td>5</td>
<td>5</td>
<td>2</td>
<td>6</td>
<td>4.8</td>
</tr>
<tr>
<td>Ferran</td>
<td>10</td>
<td>10</td>
<td>7</td>
<td>10</td>
<td>10</td>
<td>9</td>
<td>3</td>
<td>6</td>
<td>8.1</td>
</tr>
<tr>
<td>Polaris-Q</td>
<td>7</td>
<td>3</td>
<td>2</td>
<td>8</td>
<td>8</td>
<td>2</td>
<td>10</td>
<td>10</td>
<td>6.3</td>
</tr>
<tr>
<td>UF-IT</td>
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<td>3</td>
<td>6</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>7</td>
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<td>4.4</td>
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<tr>
<td>TOF</td>
<td>9</td>
<td>6</td>
<td>7</td>
<td>9</td>
<td>7</td>
<td>2</td>
<td>9</td>
<td>8</td>
<td>7.1</td>
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<tr>
<td>MG-2100</td>
<td>9</td>
<td>7</td>
<td>10</td>
<td>10</td>
<td>5</td>
<td>10</td>
<td>6</td>
<td>7</td>
<td>8.0</td>
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<tr>
<td>CDFMS</td>
<td>4</td>
<td>5</td>
<td>9</td>
<td>8</td>
<td>6</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>5.0</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td><strong>4.7</strong></td>
<td><strong>4.5</strong></td>
<td><strong>4.5</strong></td>
<td><strong>6.2</strong></td>
<td><strong>5.8</strong></td>
<td><strong>3.5</strong></td>
<td><strong>6.0</strong></td>
<td><strong>7.1</strong></td>
<td></td>
</tr>
</tbody>
</table>

1Excluding Ferran and MG-2100
Conclusions

• Various Mass Analyzer Systems Evaluated

• Several Systems Show Promise
  Stanford Research Systems RGA-100
  Inficon XPR-2
  University of Florida – Ion Trap
  Compact Double Focus Mass Spectrometer

• Areas That Need Improvement
  Response Time       Recovery Time
  System Volume      System Weight

• Future Work
  Investigate Techniques To Improve Systems
  Evaluate Engineering Challenges