Compact High Resolution QIT-Mass Spectrometers for Lunar and Planetary Applications

F. Maiwald, J. Simcic, D. Nikolic, A. Belousov, and S. Madzunkov
• Air Monitor for Human Space Explorations
  • Requirements
  • Quadrupole Ion Trap Mass Spectrometer (QIT-MS)
  • MEMS Gas Chromatography Components
  • Results on ISS
• Compact QIT-Mass Spectrometer for Lunar and Planetary Applications
  • Lunar Exospheric
  • Requirements
  • Results in Laboratory
• Future applications of frontends under development
• Conclusions
Development of Air Monitor for Human Space Explorations

• NASA instrument and JPL strategic funding for:
  • GC-QIT-MS for major constituent analyses (MCA) and trace gas analyses (TGA) for ISS cabin health monitoring
    • VCAM and S.A.M.
    • ESI-QIT-MS for exploring ocean worlds
  • QIT-MS with applications driven by sample input
    • Significant reduction in mass, power, volume, and data rate over past decade
    • Focus on TRL enhancement for flight applications and transition to commercialization

Vehicle Cabin Atmosphere Monitor (VCAM)
ISS deployment in 2010
  • Funded by NASA AEMC

Spacecraft Atmosphere Monitor (S.A.M.)
ISS power on in August 2019
  • Funded by NASA AEMC & AES
Spacecraft Atmosphere Monitor (S.A.M.) Major Requirements

### Technical Specifications

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td><strong>Mass</strong></td>
<td>9.55 kg</td>
</tr>
<tr>
<td><strong>Dimensions</strong></td>
<td>9.5&quot; x 8.75&quot; x 7.5&quot;</td>
</tr>
<tr>
<td><strong>Average Power</strong></td>
<td>42 W (28 VDC, 1.5 A)</td>
</tr>
<tr>
<td><strong>Startup Time</strong></td>
<td>&lt;2 min</td>
</tr>
<tr>
<td><strong>Configuration</strong></td>
<td>Rack-Mounted (EXPRESS), Aisle-Deployed</td>
</tr>
<tr>
<td><strong>Communication</strong></td>
<td>Wired or WiFi (aisle-deployed)</td>
</tr>
<tr>
<td><strong>Compute Element</strong></td>
<td>Xilinx Zynq FPGA (Red Pitaya)</td>
</tr>
<tr>
<td><strong>Operating System</strong></td>
<td>Linux</td>
</tr>
</tbody>
</table>

### MCA Mode: Major Constituent Analysis

<table>
<thead>
<tr>
<th>Specie</th>
<th>Measurement Range</th>
<th>Measurement Precision (for 30 s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen (N₂)</td>
<td>360 – 600 Torr (47-79%)</td>
<td>±0.66 Torr (±0.079%abs)</td>
</tr>
<tr>
<td>Oxygen (O₂)</td>
<td>130 – 160 Torr (17-21%)</td>
<td>±0.54 Torr (±0.071%abs)</td>
</tr>
<tr>
<td>Carbon Dioxide (CO₂)</td>
<td>3 – 7 Torr (0.4 – 1.0%)</td>
<td>±0.01 Torr (±0.007%abs)</td>
</tr>
<tr>
<td>Methane (CH₄)</td>
<td>0 – 7 Torr (0 - 1.0%)</td>
<td>±0.07 Torr (±0.009%abs)</td>
</tr>
</tbody>
</table>

### TGA Mode: Trace Gas Analysis

<table>
<thead>
<tr>
<th>Specie</th>
<th>Low (PPM)*</th>
<th>High (PPM)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexane</td>
<td>0.014</td>
<td>1.4</td>
</tr>
<tr>
<td>Propional</td>
<td>0.004</td>
<td>0.04</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.5</td>
<td>11</td>
</tr>
<tr>
<td>1-Butanol</td>
<td>0.02</td>
<td>0.7</td>
</tr>
<tr>
<td>Acetone</td>
<td>0.04</td>
<td>1.3</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.01</td>
<td>0.2</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.03</td>
<td>0.3</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>0.07</td>
<td>0.2</td>
</tr>
</tbody>
</table>

S.A.M. Status

- TDU#1 in operation on ISS since Sep. 2019
- TDU#2 in development for planned delivery by the end of 2020 (depending on COVID19)
Main Component of QIT-MS

- QIT-MS base pressure high $10^{-11}$ torr

- **Operates without He buffer gas**

- Different modes of operation (dynamic, static, resonant ejection)

- S.A.M. operating pressure starting at $1 \times 10^{-5}$ (collision of $N_2$) but nominal $5 \times 10^{-9}$ torr

- S.A.M. operating sensitivity $5 \times 10^{12}$ cnts /torr/sec (dynamic)

- Inlet = fused silica tube (single)

- Allows for MCA every 2 sec

Notes

QIT-MS = Quadrupole Ion Trap Mass Spectrometer
S.A.M. = Spacecraft Atmosphere Monitor (launch 2019)
MEMS Gas Chromatography Components

For S.A.M. we developed a variety of chip-based gas chromatography components that can be mixed and matched to give complete systems (or coupled to mass spectrometers) for a variety of planetary and human applications.

Pre-Concentrator (PC)
- Carboxen 1000
- ~200 μm particles
- ~10 Å pore diam.
- Heater/carboxen/inlet-outlet layers

Micro-Valve (MV)
- Four microvalves are integrated in a chip: Sample, Vent, Carrier, and Injection.
- All the valves are electrostatic.

Gas Chromatograph (GC)
- 1 m length x 86 μm diameter chip dynamically coated.
- Serpentine column is superior to spiral design.
- A novel turn geometry to counteracts the dean vortices producing lower dispersion.
- Chips can be stacked to increase column length.

Other frontend developments in progress to support analyses of water and other liquids, aerosols, and capturing molecules under hypervelocity (~10km/sec)

Miniaturization of trace gas analyzer inlet system by micromachining
S.A.M. Spacecraft Atmosphere Monitor

Flight:
- Mass: (2011, VCAM) 30 kg, (2019) 7 kg
- Power (2011, VCAM) 100 W, (2019) 30 W
- Data rate 3.2 kbits (compressed)
- Simple operation

Significant mass and power reduction for S.A.M.
Meeting measurement requirements despite sensitivity to Earth’s magnetic field

- Earth’s magnetic field observed with TDU#1
- TDU#2 will have magnetic shielding
- No impact on MCA measurements

Isotopic long term stability of S.A.M. data (adjusted to Earth reference values)

Results are comparable to magnetic-sector isotope-ratio mass spectrometers

To be published:
S. M. Madzunkov, D. Nikolić, A. Belousov, and M. R. Darrach,
“Data Analysis and Isotopic Ratios Measured Onboard the Spacecraft Atmosphere Monitor,” 50th International Conference on Environmental Systems ICES-2020-527
12-16 July 2020, Lisbon, Portugal

High stability of QIT-MS
High resolution data of QIT-MS

- High-resolution without helium buffer gas QIT-MS (unpublished)
- Xe isotopes and their ratio in air without and with resonant ejection QIT-MS (unpublished)
- Resolving 4He and D2 isobars QIT-MS (unpublished)
- C isotope ratios QIT-MS (unpublished)

Lunar Effort
Sensor

Power and CPU Electronics

Cap electronics

Integrated Software

Mechanical Integration
High Q diamond weave Litz wire coil

Dal package (fab started)
Lunar Exospheric Processes

- Observation of time variability of multi-day lunar surface exospheric and radiation changes
- Identifying and quantifying exosphere species with abundances ≥ 10 molecules/cm$^3$
  - e.g. low abundance of CO and N2; not measured before e.g. Kr, Xe
- Primary mechanism for creation of lunar exosphere are:
  - Solar wind activities with next expected maximum in 2026+/−2 years
  - Radioactive decay
  - Meteorite impact

Requirements modeled/demonstrated in the Laboratory

<table>
<thead>
<tr>
<th>Driving Measurement Requirement</th>
<th>Lunar Surface Observable</th>
<th>Instrument Performance Requirement</th>
<th>Projected Performance</th>
<th>Margin</th>
<th>To reach Xe isotopes</th>
<th>Low pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Determine which volatile species are present at the lunar surface at abundances ≥10 cm⁻³</td>
<td>H, H₂, ³He, ⁴He, Ne, N₂, O₂, Ar, CH₄, CO, CO₂, Kr, Xe, OH, H₂O</td>
<td>Mass Range (Da)</td>
<td>1-140</td>
<td>0.75-230</td>
<td>65%</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mass Resolution (m/Δm FWHM)</td>
<td>200</td>
<td>1000</td>
<td>400%</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Sensitivity (molecules/cm³/sec)</td>
<td>0.001</td>
<td>0.0005</td>
<td>100%</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Target species partial pressure (Torr), 2:1 SNR</td>
<td>≤1 × 10⁻¹⁴</td>
<td>≤1.3 × 10⁻¹⁵</td>
<td>700%</td>
<td></td>
</tr>
</tbody>
</table>

Sources used in compiling the required LUNAR targets are:

1) 2013-2022 Planetary Decadal Survey, Visions & Voyages, p. 118, critical science goal for the moon and other inner solar system bodies: "Understand the Composition and Distribution of Volatile Chemical Compounds…"

2) 2007 NRC Report: Scientific Context for Exploration of the Moon

8a. Determine the global density, composition, and time variability of the fragile lunar atmosphere before it is perturbed by further human activity.

8c. Use the time-variable release rate of atmospheric species such as ⁴⁰Ar and radon to learn more about the inner workings of the lunar interior.

8d. How water vapor and other volatiles are released from the lunar surface and migrate to the poles where they are adsorbed in polar cold trap.

3) LEAG Specific Action Team Report. Goal 8a: “Systematically detect trace volatile species, like water, OH, and hydrocarbon in the exosphere.”

4) LEAG Specific Action Team Report. Goal 8b: “Detect volatile transport from mid- to high-latitudes as a function of driving space environmental (solar storm, meteor stream) conditions.”
https://www.lpi.usra.edu/leag/reports/vsat_report_123114x.pdf

https://www.nasa.gov/sites/default/files/atoms/files/leag-gap-review-sat-2016.pdf
Isotope spectra of a sample of calibrating gas (1.7E-10 Torr of Kr and 1.3E-11 Torr of Xe) measured continuously for 7 hours yielded a 0.6 ‰ precision on the 86Kr/84Kr ratio.

Sensitivity of QIT-MS is better than 1% of Xe isotopic ratios.
Predicted QIT-MS Response at Lunar Surface (diurnal)

Simulation results with JPL lunar model (based on previously published in peer reviewed journals)


Lunar exosphere model based on past measurements with LADEE is detectable with QIT-MS.

Approx. 30% higher counts during sun exposure (lunar day)
Modelled and Measured High Resolution Mode

Measured and Modeled QITMS Mass Spectra

(Left) Measured QITMS spectra for 4He and D2 (dotted line) with a modeled 4He and D2 spectra.

(Right) Modeled spectra for 3He and HD, at identical abundances, for various RF frequencies. The equal 3He and HD abundances are based on the published isotopic ratios in the lunar regolith [Wiens (2003)] and the expected AtLAS H2 instrument off-gassing after < 1 day of lunar surface bakeout.


Well validated QIT-MS model.
Future Efforts
Future applications of frontends under development (1/2)

**Advanced Aerosol Separator for PM2.5 Particles** (proposal phase)

- Instrument design concept and model completed
- Continuous regulation of input flow with piezo controlled orifice (up to 100 bar, operating up to 150°C, response time in the order of msec)
- Analyses of suspended aerosol particles at ppb levels by focusing along the flow axis
- Collaboration with Integrated Deposition Solutions (IDS) for NanoJet development
- Enabling real-time monitoring of aerosol particles in ambient gas
  - Venus decent
  - human habitats

The Aerosol Separator has a differentially pumped flow chamber (1) designed as a sample inlet to any mass spectrometer. The major components are a NanoJet Flow Cell (2), relaxation cell with the cyclone separator (3), micropirani pressure gauge (4), internal (5a) and external (5b) vacuum ports, and non-corrosive 3D-printed vacuum chamber (6). The prototype will use a Pfeiffer HiCube 80L/s Eco pump system, a 200 amu RGA from the Stanford Research Systems (SRS), and LOAC optical particle counter/sizer is an optional module currently being built under JPL/CNES collaboration.

References:

David Keicher, Marcelino Essien, Fa-Gung Fan, Nicolas Verdier, Jurij Simcic, and Dragan Nikolić, "Advanced Aerosol Separator for PM2.5 Chemical Composition and Size Distribution Analysis," 50th International Conference on Environmental Systems ICES-2020-351 12-16 July 2020, Lisbon, Portugal, to be published

Future applications of frontends under development (2/2)

- The Ocean Worlds Life Surveyor (OWLS) is funded under the JPL NEXT Program initiated in 2018.
  - Goal to build and field test (Borup Bjord Pass in the Canadian High Arctic) prototypes in preparation to select instruments for possible missions to Enceladus, or Europa

- Mass Spectrometer is part of Organic Capillary Electrophoresis Analysis System (OCEANS)
  - Electrospray Ionization coupled to Mass Spectrometry (ESI-QIT-MS) for broad-based detection and characterization of collections of organic molecules.
  - Detection of organics at ppb level, with expected accuracy of 2% for relative amino acid abundances.

- Life detection hinges upon identifying certain organic molecules
  - Amino acids are the building block of proteins and their distribution provide distinct biosignatures.

- Prototype of ESI system is ready for testing with laboratory setup and MS in near future

- https://microdevices.jpl.nasa.gov/capabilities/in-situ-instruments-chemical-analysis/owls-project/
Conclusions

• Preparation for Lunar application started with DALI program.
  • Further reduction in mass (< 7kg) and power (<30W)

• QIT-MS accuracy/precision matches with laboratory size magnetic sector MS at shorter integration times

• Proposing for near-future flight opportunities to raise the TRL level
  • Discovery and New Frontiers
  • Instrument developments
  • Internal funding

• Future work will focus on sample inlets designs to target different NASA missions
  • Development on Electro-Spray frontend for liquid sample
  • Investigations of an aerosol separator for high density atmospheres by utilizing the newly developed piezo controlled valve for constant input flow during decent
Thank you for your attention!

Questions?
Meet the Core Team

Typical Education
- Physics
- Chemistry
- Electronics
- Geoscience

Experience
- Physics and Chemistry
- Theory and modelling
- Instrument development
- Publications and proposals
- Teamwork