National Aeronautics and Space Adminstration

FY24 Strategic Initiatives Research and Technology Development (SRTD)

Quadrupole Ion Trap Mass Spectrometer (QITMS) for the Supercritical CO2 and Subcritical H2O Analysis instrument (SCHAN)

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Strategic Focus Area: In-Situ Extant Life Detection Technology I **Strategic Initiative Leader:** Victor S Abrahamsson

Objectives: The objective of this task was to develop an ion transport interface between the Supercritical CO2 and Subcritical H2O Analysis (SCHAN) frontend and the JPL Quadrupole Ion Trap Mass Spectrometer (QITMS). **Problem:** The ion source of SCHAN creates ions at ambient pressure, while the QITMS operates at a 7 orders of magnitude lower pressure. **Solution:** Develop an ion transport assembly (ITA), an ion optics interface enabling ion transport through multiple vacuum stages.

FY 24 Objectives:

(1) Prove that fast ions from a linear guiding quadrupole can be loaded into a QITMS trap

(2) Develop a compact brassboard assembly with three pressure stages, building on lessons learned from the breadboard design utilized in year 1 and 2.

Background: The SCHAN instrument is using water and CO2 at low temperatures to extract microbial biosignatures at ppt concentration levels. The detection of those is done through electrospray ionization mass spectrometry. On Earth, this is facilitated by buffer gas to slow ions down to enable loading them into a mass spectrometer. However, carrying the amount of buffer gas necessary for extended life detection missions in space is untenable; thus the need for an interface allowing the direct and efficient (~1% of generated ions) transduction from ambient-pressure electrospray ions into a unbuffered high-vacuum mass spectrometer.

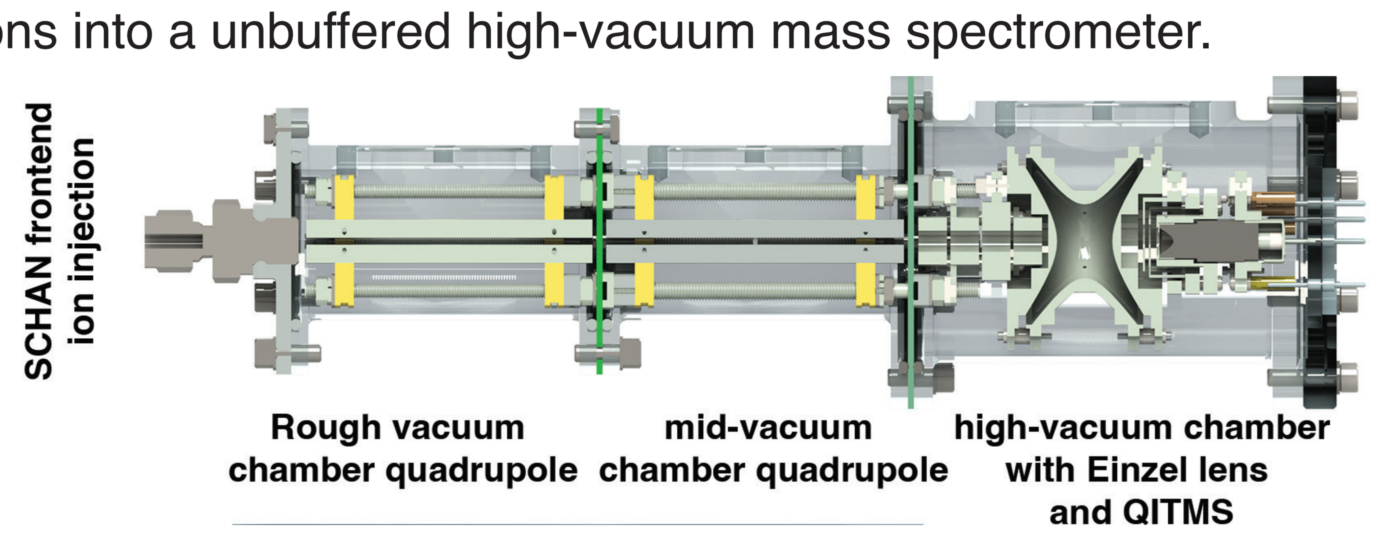


Figure 1. SCHAN-QITMS ion transport brassboard assembly. Ambient pressure ions are ejected by the frontend ESI and caught and guided through two linear quadrupoles, passing through the novel circuit board chamber dividers that double as electric interfaces for the quadrupoles and as pinholes. An ion lens then focuses the ion beam into the QITMS, where they are analyzed.

Significance/Benefits to NASA: The initial proof of QITMS loading without buffer gas fundamentally allows tankless mass spectrometer operation, only limited in consumables by the ion source frontend. Although scheduling and funding constraints prevented full integration and testing of the brassboard design (Fig 1), the RGA-QITMS proof of concept suggests that buffer gas is not required for successful loading, and that future versions of the QITMS may not need to rely upon consumable buffer gas reservoirs.

The long-term benefits for JPL will be the development of a fully integrated and compact interface and mass spectrometer for future in situ space missions dedicated to the search for organic molecules and biosignatures.

Approach and results: Without buffer gas, detecting ions becomes more challenging because they can have higher kinetic energy and more erratic motions. Our approach to high vacuum QITMS relies on precise radiofrequency (RF) fields to trap ions and control their motion. By carefully adjusting the electric fields, the system can still confine and manipulate a modest number of ions long enough for mass analysis.

Subtask (1) The breadboard assembly from previous years could successfully guide electrosprayed ions into the high vacuum chamber, but not into the small QITMS entrance pinhole, due to inherent alignment challenges. Thus, an independent proof-of concept for feasibility of high vacuum ion trap loading was devised: A commercial off-the-shelf (COTS) residual gas analyzer (RGA) ionizer and linear quadrupole was coupled with the JPL QITMS to show whether vacuum ions can be trapped and detected.

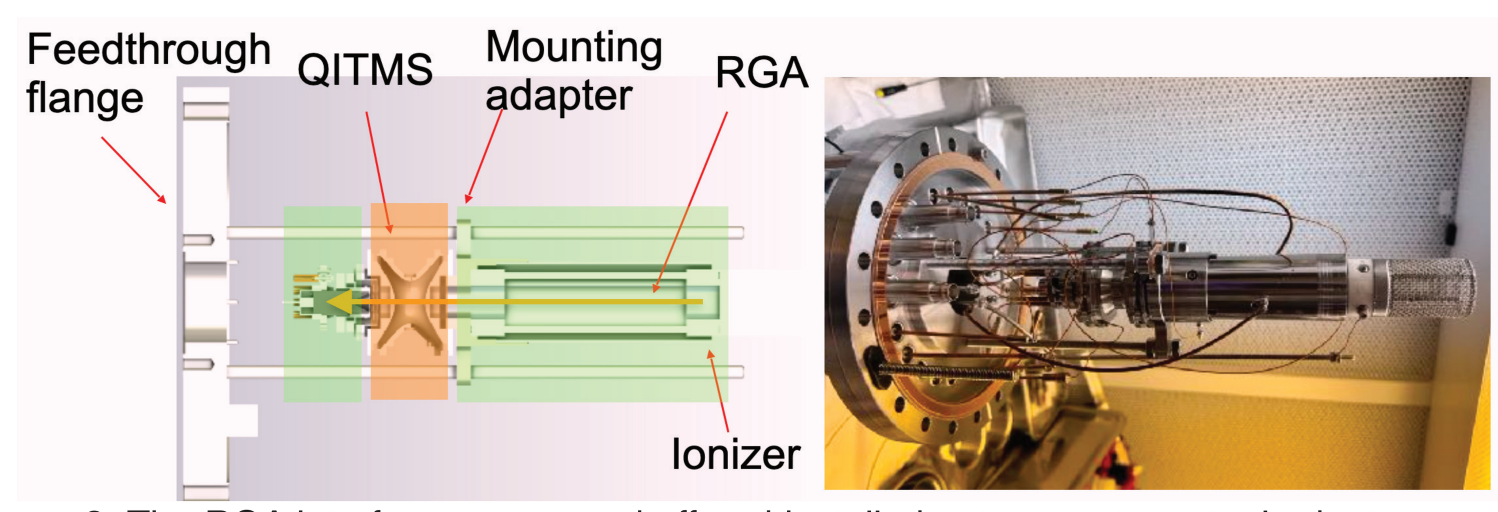
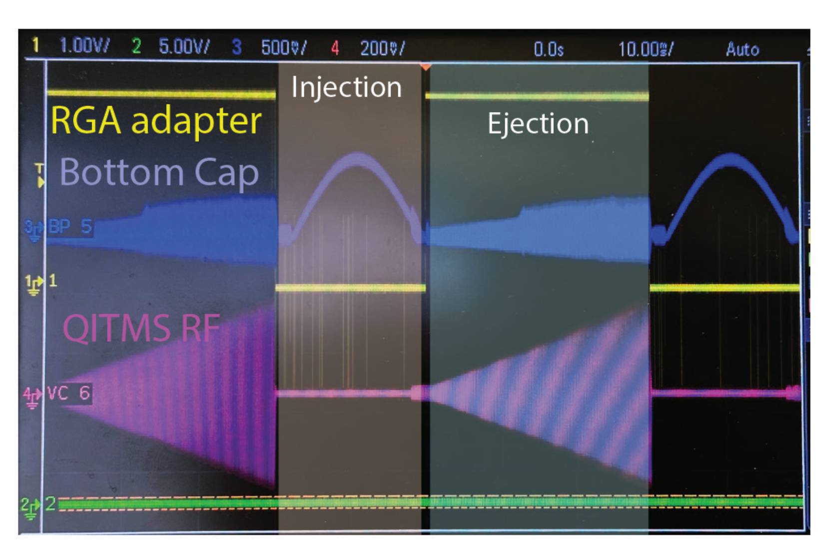


Figure 2. The RGA interface was sawed off and installed onto a custom steel adapter assembly, designed to align the RGA quadrupole ion outlet perfectly with the QITMS ion inlet aperture, with RGA electrical connections rerouted in a way to minimize capacitive coupling of the linear quadrupole RF. Despite the massively off-label implementation, a mass range from 1 to 78 amu on an 100 amu RGA was retained.

The QITMS was successfully activated in this setup (Fig. 2), trapping just below 0.1% of the ions delivered by the RGA ionizer and quadrupole. While missing the target of 1%, this still proves that modest ion trapping without buffer gas is feasible (Fig. 3).



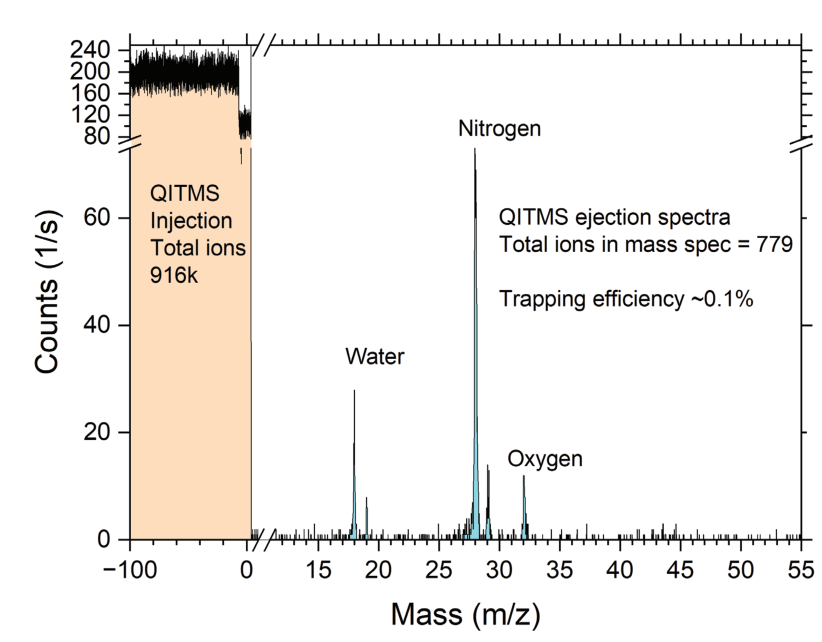


Figure 2. QITMS injection/scan frame sequence (left). The RGA adapter is grounded, letting ions from the RGA linear quadrupole pass (flashes in yellow line). The bottom cap repelling potential (blue line) can be modulated with a gated arbitrary wave generator. For ejection, incoming ions from the RGA are blocked with a high adapter plate potential, and the RF amplitude is ramped, ejecting heavier ions with increasing amplitude. **QITMS mass spectra (right)**. The graph shows the bypassing ion count during injection cycles, and the mass spectra of the trapped ions during ejection phase, with a trapping effiency of ~0.1%.

Subtask (2) The brass-board design drafts inherited from former staff was modified to make them manufacturable. Three vacuum stage chambers were completely redesigned to allow billet manufacturing rather than expensive metal 3D-printing ($25k/chamber vs $9k/chamber). All designs were cleaned up and documented in EPDM, all parts necessary for assembly were manufactured and are in stock, aside from circuit board vacuum dividers and some small internal parts. The assembly and end-to-end testing were not achieved due to cost overrun before the end of the task.

Figure 4. Selection of manufactured and available brassboard SCHAN-QITMS parts

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