The Technology Demonstration of the Spacecraft Atmosphere Monitor

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The Spacecraft Atmosphere Monitor (S.A.M.) is a miniaturized Gas Chromatograph Mass Spectrometer (GC/MS) instrument being sent to the International Space Station (ISS) in 2019. While on-station, the S.A.M. instrument will continuously monitor the major atmospheric constituents as well as trace organic volatiles in the cabin air daily. At its core, the S.A.M. sensor consists of a quadrupole ion trap mass spectrometer (QITMS) coupled to a MEMS preconcentrator, gas chromatograph, and microvalve system. Its miniature, ruggedized form factor allows the S.A.M. to be aisle-deployed throughout different nodes of the ISS to monitor different astronaut environments and activities such as exercise and sleep. The final system design of the S.A.M. flight unit, regarding the GC/MS architecture, the mechanical and electrical assembly, and the software implementation, is discussed in detail and the S.A.M. flight unit performance is presented.

Nomenclature

S.A.M.	=	Spacecraft Atmosphere Monitor
GC/MS	=	Gas Chromatograph Mass Spectrometer
ISS	=	International Space Station
QITMS	=	Quadrupole Ion Trap MS
MEMS	=	Micro-Electro-Mechanical Systems
VOC	=	Volatile Organic Compound
TDU	=	Technology Demonstration Unit
DM	=	Development Model
MSFC	=	Marshall Spaceflight Center
VCAM	=	Vehicle Cabin Atmosphere Monitor
MCA	=	Major Constituents Analysis
TGA	=	Volatile Organic Compound
PCGC	=	Preconcentrator Gas Chromatograph
HIM	=	Human Interface Module
CEM	=	Channel Electron Multiplier
SRL	=	Series Resonant Inductor
NEG	=	Nonevaporable Getter
MDV	=	Mindrum Valve
MV	=	Microvalve
FPGA	=	Field Programmable Gate Array
MSRFA	=	MS Rigid Flex Assembly
VHCE	=	Valve Heater Control Electronics
ECB	=	Endcap Board
AHVPS	=	Adjustable High Voltage Power Supply
ECLSS	=	Environmental Control and Life Support System

I. Introduction

THE Spacecraft Atmosphere Monitor (S.A.M.) is a technology demonstration of a highly-compact gas chromatograph mass spectrometer (GC/MS) instrument for measuring the major constituents and trace volatile organic compounds (VOCs) in the cabin air of the International Space Station (ISS) and future crewed vehicles. Over the past three years, the S.A.M. instrument has been developed, matured, and tested using a step-wise methodology. Previous reports discussing the progress towards the S.A.M. Technology Development Unit (TDU) can be found elsewhere[1,2,3]. During the development phase, the instrument has advanced in maturity and capability through two Development Models (DM1 and DM2). Throughout the development of S.A.M., the environmental test facilities at Marshall Space Flight Center (MSFC) were used to test the performance of the DM units. Results from this testing have been used to inform the S.A.M. project through its maturation to the TDU, which will be operated and validated

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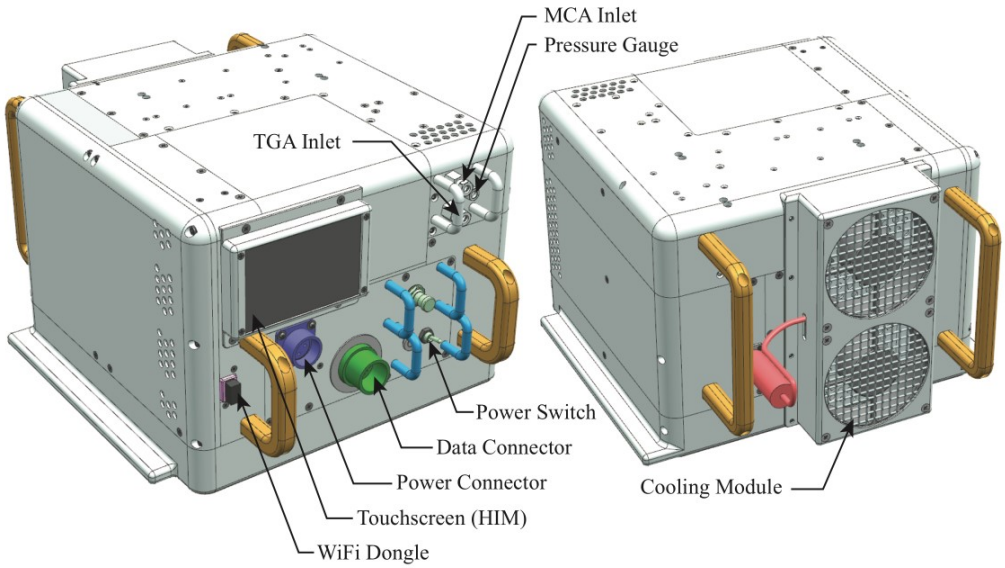

Figure 1. The S.A.M TDU. *Front and rear perspectives of the S.A.M. TDU showing the various front panel interfaces and the rear cooling module. The aluminum chassis is 9.5" x 8.75" x 7.5" in volume and weighs approximately 10 kg. The S.A.M. handles and small form factor allow for the instrument to be easily transported to perform cabin-air monitoring in either an aisle-deployed or a rack-mounted configuration.*

aboard the ISS in 2019. In this paper, the system design and performance of the S.A.M. TDU is presented and the plan towards its deployment to the ISS is discussed.

II. Instrument Overview

The S.A.M. TDU, shown in Figure 1, is a direct successor of the VCAM instrument[4,5,6] which operated for two years onboard the ISS. Although VCAM and S.A.M. provide similar functionality, the S.A.M. TDU incorporates several key technological advances including 1) the use of a passive pumping system (an ion/getter pump) rather than turbo and roughing pumps; 2) nominal operation under high vacuum conditions during trace gas measurements; 3) and the introduction of MEMS components. These advances enable the S.A.M. instrument to operate under one half of the VCAM power consumption in a compact form factor which is one third of VCAM mass and volume. Because of its small size, the S.A.M. TDU can be remotely operated in an aisle-deployed configuration throughout the ISS. Otherwise the instrument will be stowed in a rack-mounted locker configuration located in an ISS EXPRESS rack (EXpedite the PRocessing of Experiments for Space Station). For a technical comparison of VCAM and S.A.M. regarding functionality and instrument specifications, see Reference 1.

On-station, the S.A.M. instrument is tasked with monitoring both the major constituents (N_2, O_2, CO_2, CH_4) and certain trace VOCs (listed in Table 1) for one year. The primary mode of S.A.M. operation is Major Constituent Analysis (MCA), during which a small air leak into the QITMS is opened allowing the cabin-air to be passively sampled and continuously monitored. The secondary mode, Trace Gas Analysis (TGA), will be initiated on a daily basis or on-demand under special circumstances. During TGA, the cabin-air is actively sampled through a preconcentrator gas chromatograph (PCGC) front-end to provide chemical gain and separation prior to analysis in the QITMS. The S.A.M. system level technical specifications regarding MCA and TGA operation and performance are also listed in Table 1.

The S.A.M. instrument volume (10.2 L), defined by its chem-filmed aluminum chassis, is 9.5" by 8.75" by 7.5" and designed to withstand the high-G loads during launch. The instrument is convectively cooled using a removeable cooling module which is attached to the rear of the device. The front panel of S.A.M. includes the power, data, and WiFi connectors, the power switch, and various inlets for cabin-air monitoring. Although the S.A.M. TDU is predominantly autonomous, the front panel also includes a touchscreen, or Human Interface Module (HIM), enabling astronaut control of low-level operations such as initiating different operational modes such as Standby, MCA, or TGA. In total the instrument weighs 10 kg and has an average power draw of 45 W.

Table 1. S.A.M. Technical Specifications for MCA and TGA. *Key parameters regarding science performance of the S.A.M. TDU GC/MS during different modes of operation. Note that values marked with * are expected TDU values. All low and high levels for trace gas detection are based on S.A.M. requirements.*

MCA Mode		
Report Cadence	2 s	
Data Integration Time	10 s	
Leak Description	1.5" x 2 µm ID microcapillary	
Leak Rate	5 x 10^{-8} Torr L/s	
QITMS Pressure	10^{-9} – 10^{-8} Torr	
Species	Measurement Range	Measurement Precision (for 10 s)
Nitrogen (N_2)	360 – 600 Torr (47-79%)*	±0.5 Torr (±0.07%)
Oxygen (O_2)	130 – 160 Torr (17-21%) *	±0.5 Torr (±0.07%)
Carbon Dioxide (CO_2)	3 – 7 Torr (0.4 – 1.0%)	±0.1 Torr (±0.01%)
Methane (CH_4)	0 – 7 Torr (0 – 1.0%)*	<±0.5 Torr (±0.03%)*

TGA Mode					
Frequency			1 per day (or on-demand)		
Run Time			10 – 20 minutes		
GC Carrier			H_2 (10 L metal hydride tank)		
GC Column			6 m x 86 µm ID microcolumn		
GC Flow rate			0.10 sccm H2		
PC Description			250 nL Carboxen 1000		
PC Heating			250 ºC for 5 s		
QITMS Pressure			10^{-6} – 10^{-5} Torr		
TGA Measurement Precision			40% relative		
Species	Low (PPM)*	High (PPM)*	Species	Low (PPM)*	High (PPM)*
Hexane	0.014	1.4	Dichloromethane	0.01	0.1
Propenal	0.004	0.04	Acetaldehyde	0.06	1.1
Ethanol	0.5	11	Perfluoropropane	13	130
2-Propanol	0.04	4	Methanol	0.1	4
1-Butanol	0.02	0.7	Octamethylcyclotetrasiloxane	0.02	0.2
Acetone	0.04	1.3	Hexamethylcyclotrisiloxane	0.02	0.2
Benzene	0.01	0.2	Decamethylcyclopentasiloxane	0.01	0.1
Toluene	0.03	0.3	Propylene glycol	TBD	TBD
o,m,p-Xylene	0.02	0.2	Trimethylsilanol	0.05	1

III. Description of the S.A.M. Subsystems

Located inside the S.A.M. mechanical structure are the QITMS assembly, the PCGC assembly, and printed circuit boards (PCBs) which make up the electronics assembly. The PCGC assembly is built onto a section (or "slice") of the S.A.M. chassis which holds pressurized gas lines, vacuum valves, and filters that feed sampled air and hydrogen carrier gas into the MEMS PCGC subassembly and ultimately into the QITMS assembly. The QITMS assembly consists of a titanium vacuum chamber which houses the QIT sensor and ion/getter pump. In this section, the composition and functionality of these subsystems are described in detail.

A. The Quadrupole Ion Trap Mass Spectrometer

The S.A.M. QITMS, shown in Figure 2, consists of four main components: the gas inlet system, the electron gun, the miniaturized QIT, and the channel electron multiplier (CEM) detector subassembly. The entire assembly as whole is a compact, "wireless" design to minimize its size and to reduce potential complications with internal wire-routing. The assembly is approximately 120 mm in length and 70 mm in diameter. Typical sensitivities of the S.A.M. QITMS are on the order of 10^{12} Hz/Torr but can be increased up to 10^{14} Hz/Torr for certain operating conditions.

The gas inlet system consists of two 1/16" OD x 0.040" ID stainless steel tubes which are fed from the TGA and MCA transfer lines through a custom titanium conflat flange into the trap volume of the QITMS. The TGA line is treated with a silicon-barrier coating (Silcoguard by Silcotek[7]) to prevent adhesion of sampled trace organics which might lead to cross contamination between TGA runs. The custom titanium conflat flanges (MPF[8]) have a minimal thickness of 0.25" and include a brazed alumina insert with embedded electrical feedthroughs where the QITMS voltages are applied.

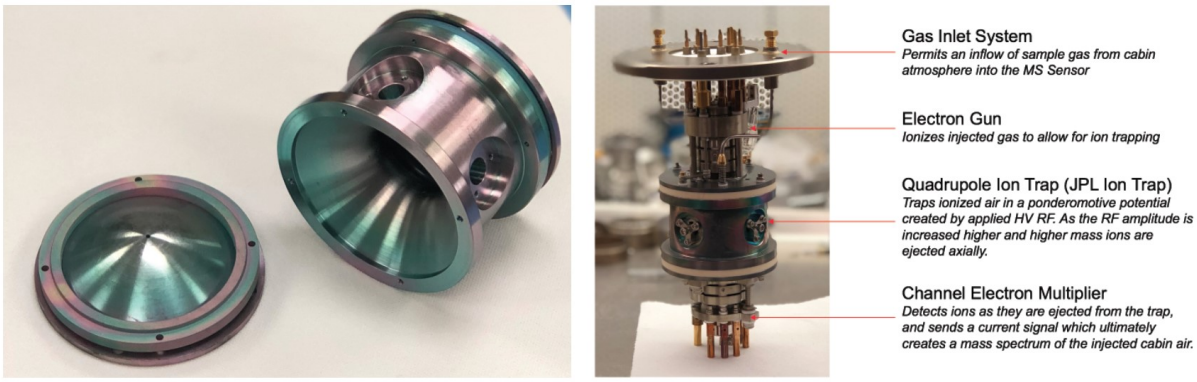

Figure 2. The S.A.M. QITMS. *The Silcoguard-coated 10 mm QIT (left) is based on the JPL Ion Trap which has been used for multiple MS applications. The QITMS subassembly (right) contains the gas inlet system, the electron gun used for electron-impact ionization, the JPL ion trap, and the channel electron multiplier.*

The electron gun used to ionize the sampled gas is composed of a tantalum disc filament (ES-042 by Kimball Physics[9]), a cathode and anode electrode, and an Einzel lens used to focus the axially-introduced electron beam at the QITMS trap center. Under nominal operating conditions, the emission current is measured to be 40 μA with a beam energy of 70 eV. While the QITMS duty cycle is routinely varied, a nominal 50 Hz duty cycle includes a 10 ms ionization period which generates up to 1000 trapped ions (depending on trap pressure).

The QIT used in the S.A.M. QITMS is a 3D Paul Trap with a 10 mm field radius and effective capacitance of 85 pF. The trap is nominally operated using an 800 kHz rf voltage up to 2 kV in amplitude provided by a series resonant inductor (SRL) to the central ring electrode. The top and bottom endcaps are nominally kept at ground but, if desired, can be driven with arbitrary rf (180º out-of-phase) to provide secular excitation profiles to the trapped ions for further mass discrimination. These ion trapping parameters correspond to mass ranges up to 330 amu. At the center of both endcaps are two 1 mm OD x 2.5 mm long holes: one for the introduction of the electron beam and the second for the ejection of ions into the detector assembly. These small axial orifices have the added effect of transforming the trap volume into a pressure cell due the small 0.1 L/s effective conductance between the trap volume and the external vacuum chamber. Typical pumping speeds in the external chamber (~10 L/s) result in a 100-fold increase in pressure (and therefore ion count rates) in the QITMS trap volume. To prevent the creation of patch potentials due to the adhesion of trace organics on trap surfaces, the QIT is also coated with Silcoguard. To further maintain the cleanliness of trap surfaces, the QITMS is equipped with a 20 W halogen bulb which nominally heats the trap to above 200 ºC.

The QITMS detector assembly consists of a CEM (5901 Burle Magnum[10]) and two protection meshes called grids. During the ionization period of the QITMS duty cycle, the two grids are elevated to -100 V and +100 V to prevent the negatively charged electron beam and positively charged ions from striking the CEM, which could otherwise result in decreased lifetimes due to oversaturation. During the q-scan rf ramp, both grids are lowered to ground allowing ejected ions to reach the CEM. Under nominal operation, the CEM is biased to -2.2 kV. Ion count rates are corrected for non-paralyzable dead times characteristic of this CEM type (~10 ns).

The QITMS assembly is housed in a 3D-printed titanium vacuum chamber (shown in Figure 3), which is intentionally designed to minimize the weight and footprint of the MS Sensor assembly. The additive manufacturing process (CalRAM[11]) includes a state-of-the-art laser sintering procedure followed by hot isostatic pressing which reduces the porosity of the titanium to minimize outgassing and to increase its durability. After printing, the chamber undergoes traditional machining to clean out the internal volume as well as to create the knife edges for conflat flange seals. Ultimately these custom QITMS chambers exhibit external leak rates less than 10^{-11} Torr L/s and base pressures less than 10^{-10} Torr following a typical 24-hour bakeout at 150ºC.

In addition to the QITMS itself, the vacuum chamber houses a large nonevaporable getter (NEG) pump coupled with a noble diode ion pump, which are used in tandem to achieve chamber pressures 10^{-9} to 10^{-8} Torr during MCA and 10^{-6} to 10^{-5} Torr during TGA. The NEG pump is a custom SAES Getters CapaciTorr D200 cartridge[12] modified to interface with the S.A.M. chamber and to withstand the high-G loads during launch. The NEG pump consists of 25 stacked ZrVFe discs which have a cumulative mass and surface area of 28 g and 238 cm^2, respectively. The NEG pump's large hydrogen sorption capacity (280 Torr L) and pumping speed (200 L/s), permits the use of relatively high flow rates of hydrogen carrier gas (0.1 sccm) into the QITMS chamber while performing GC/MS. The noble diode

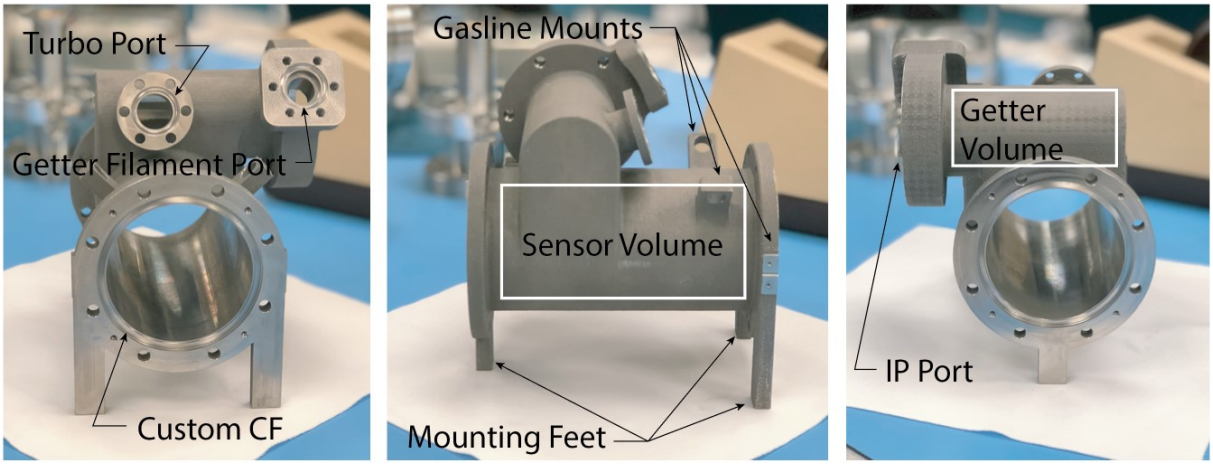

Figure 3. 3D-printed titanium QITMS vacuum chamber. *Multiple perspectives of the QITMS vacuum chamber showing the QITMS sensor and getter volumes as well as the various vacuum ports. The chamber weighs 780 g and has approximate cubic dimensions of 5" x 5" x 4". Following a 24-hour, 150ºC bake out the base pressure is measured to be <10^{-10} Torr using an activated NEG/ion pump.*

ion pump is custom manufactured by UTC Aerospace Systems[13] for spaceflight applications with a 2 L/s pumping speed over a wide range of pressures (10^{-9} to 10^{-4} Torr).

The dominant S.A.M. operational mode in terms of daily duty cycle is MCA, which is engaged continuously except for daily TGA runs (less than 1 hour) and routine power downs to transition between the rack-mounted and aisle-deployed configurations. During MCA, cabin-air is passively sampled through the MCA inlet on the front panel of the S.A.M. where it then flows directly into the QIT volume where it is analyzed. The MCA inlet line, installed in the PCGC assembly, is shown schematically in Figure 4. The flow restriction is created by a 2 µm ID x 1.5" long polyimide-coated, silica microcapillary which exhibits a 5.0 x 10^{-8} Torr L/s steady-state flow of atmosphere into the QITMS. To protect the microcapillary from dust-clogs, a replaceable 0.5 µm frit[14] is integrated into the MCA inlet. A double-latching solenoid valve manufactured by Mindrum[15] located on the vacuum-side of the microcapillary (MDV4 in Figure 4) is used to stop the influx of cabin-air in order to perform background measurements of the QITMS. The entire MCA inlet and transfer line is wrapped in heater tape and insulation to keep the metal tubing at 50ºC to minimize the adsorption of water which would otherwise result in lags in S.A.M. response times to changes in cabin humidity levels.

B. The MEMS Preconcentrator Gas Chromatograph Front-End

A unique feature of S.A.M. is the MEMS PCGC front-end to the QITMS which enables the detection of trace VOCs down to PPB concentration levels (Table 1) using an extremely small footprint in terms of space and power consumption. At the core of this subsystem is the Vespel PCGC package (Figure 5d) which contains the microfabricated preconcentrator (PC), gas chromatograph (GC) microcolumn, and microvalve (MV) chips – each approximately 15 mm x 15 mm x 4 mm. The PC (Figure 5b) is composed of a silicon heater and a 250 nL chemical trap filled with 80-100 mesh Carboxen 1000 spheres (Sigma-Aldrich[16]) which serve as the chemical gain element. During TGA, cabin air is sampled through the PC where trace VOCs adsorb to the Carboxen. Following a variable sampling time, the PC is flash-heated by applying ~20 W of power to the heater for 5 s resulting in nominal temperatures of 250 ºC (measured by monitoring the resistance of the heater element). This heating abruptly drives off the adsorbed VOCs which are then flushed into the GC microcolumn and ultimately into the QITMS resulting in chemical gains on the order of 1000, making PPB concentration relatively straightforward to detect[17].

The GC microcolumn, which provides chemical separation to simplify trace VOC detection in the QITMS, is composed of six bonded silicon wafers – each containing etched serpentine columns 1 m in length with hydraulic diameters of 86 µm (Figure 5c) – giving a total column length of 6 m. Nonpolar OV-5 coating is used for the stationary phase and is prepared using a custom in-house procedure. To reduce retention times for nonpolar VOCs, the GC chip is equipped with a foil heater which is heated to 100 ºC during the latter half of the chromatogram. Nominal hydrogen

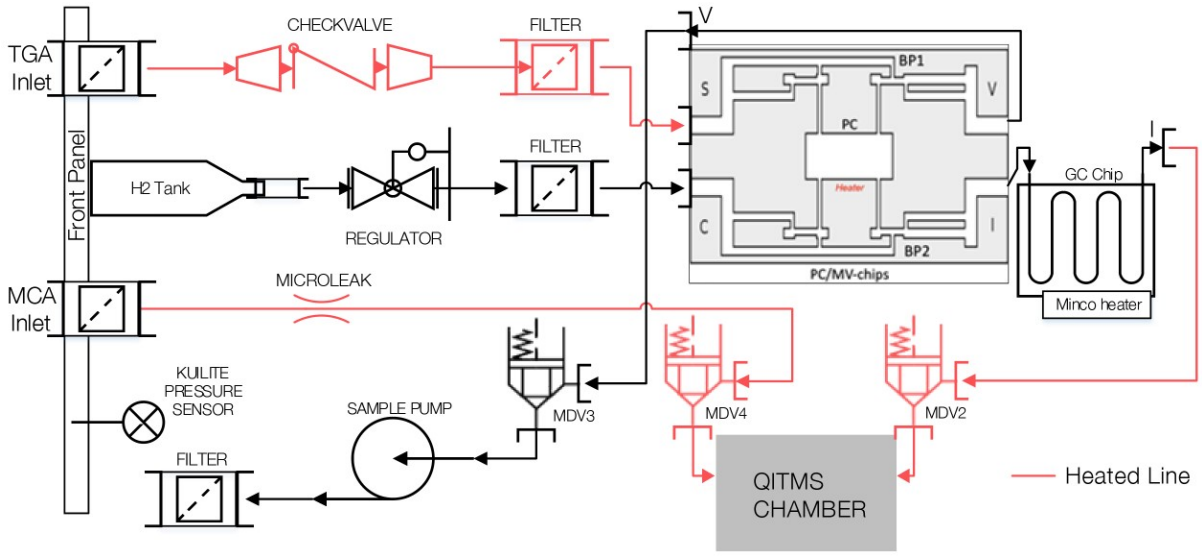

Figure 4. PCGC assembly plumbing diagram. *This schematic shows the components including filters, valves, heaters, and plumbing used in the PCGC assembly. The main paths, starting from the left side, are the sample, carrier, and MCA flow paths. Two Mindrum valves, MDV2 and MDV4, control the gas flow from the GC chip and MCA microleak to the QITMS chamber. A simplified 2-D model of the MV chip shows the various flow paths combining the input from the H2 tank and the TGA inlet during TGA runs.*

carrier head pressures are between 16 and 18 PSIa resulting in the flow rates of ~0.1 sccm and total elution times of up to 20 min for siloxanes.

Carrier and sample flow directions within the PCGC package are controlled by the MV chip. Within the MV chip are *four* independently controlled electrostatic membrane microvalves – one for the sample inlet, carrier inlet, sample outlet, and carrier/injector outlet (shown schematically in Figure 4 and realistically in Figure 5e). The MV chip itself is composed of five main layers which are shown, in addition to the PC layers, in Figure 5a. The top 2-layer pair (TCAP and VC) and bottom 2-layer pair (BCAP and VO) are each gold-diffusion-bonded silicon wafers which enclose the various etched paths leading to the PC and GC chips. Between these 2-layer pairs is a 2 µm membrane layer which is bonded to the top and bottom 2-layer pairs using a benzocyclobutene adhesive. The membrane layer contains four gold foil electrodes (one for each microvalve) insulated by a polyimide film. In normal operation, the VC and VO layers on either side of the membrane are held at 150 and 0 V, respectively, creating an electric field . To actuate an individual membrane microvalve, 150 V (or 0 V) is applied to one of the gold foils causing that portion of the membrane to flex towards the bottom VO (or top VC) layer of the MV chip. This flexing, depending on direction, opens or restricts different internal flow paths which allows cabin-air to be sampled through the PC chip or carrier gas to push desorbed VOCs into the GC chip following PC heating. Sample (green) and carrier (red) flow patterns through the MV and PC chips are shown in Figure 5e for four different membrane valve configurations that are used during various steps in the TGA sequence (sampling, injection, chromatography, and cleaning/sweeping).

The entire plumbing diagram for the PCGC subsystem is shown in Figure 4. The source of hydrogen carrier gas is a custom 4" metal hydride canister (HCI[18]) which holds 10 L of hydrogen with a head pressure of ~50 PSIg when full. An inline regulator reduces the pressure to the nominal 16 to 18 PSIa carrier pressure for chromatography (0.1 sccm). When TGA is not being performed, the MV chip is unpowered leaving the individual membrane valves in an undefined state. As a result, the hydrogen carrier gas can freely pressurize the entirety of the PCGC plumbing. To prevent the loss of hydrogen, a check valve and a Mindrum valve (MDV3) are employed behind sample inlet and before the micropump (used to draw cabin air into the PC chip during sampling), respectively. The pressurization of the PCGC subsystem with hydrogen has the added benefit of hydrodynamically checking any small air leaks. In short, the introduction of atmosphere into the PCGC plumbing while the MV chip is unpowered can lead to air filling the GC microcolumn, which poses the risk of saturating the NEG pump due its small nitrogen capacity (0.6 Torr L) when Mindrum valve 2 (MDV2) is opened during TGA. The steady-state flow of hydrogen, while not in TGA mode, is measured to be much less than 0.01 sccm which, after 1 year of operation, leads to a loss of at most 6.7 L of hydrogen.

The hydrogen flow used during the 365 daily 20 min TGA runs (0.1 sccm flow) leads to a 1.0 L loss of hydrogen. This consumption conservatively amounts to less than the 10 L supply of hydrogen included in the S.A.M. TDU.

A typical S.A.M. TGA sequence to be run each day can be broken into six phases: 1) precleaning, 2) sampling, 3) hydrogen sweeping, 4) injection, 5) hydrogen backfilling, and 6) postcleaning. During the precleaning phase, hydrogen is pulled through the PC chip by the micropump ("cleaning/sweeping" in Figure 5e). The PC is flash-heated, desorbing VOCs that may have adsorbed to the Carboxen since the previous TGA run which are then flushed from the PCGC lines by the hydrogen flow. After precleaning is complete, the 10 minute sampling phase begins ("sampling" in Figure 5e). The flow path through the MV chip is changed to stop the hydrogen flow through the PC chip and to begin to draw cabin air from the sample inlet after the pressure gradient created by the micropump opens the check valve (0.3 PSI). Once sampling is complete, residual unadsorbed air is purged from the PC chip by again redirecting the hydrogen flow through the PC chip during the sweeping phase ("cleaning/sweeping" in Figure 5e).

Throughout these initial steps MDV2 remains closed, allowing S.A.M. to continue to produce MCA data. Once the sweeping phase is complete, however, the S.A.M. QITMS is shut off (ceasing MCA) and MDV2 is opened, allowing hydrogen to flow through the 6 m microcolumn into the QITMS chamber, resulting in a large increase in chamber pressure from 10^{-9} to 10^{-5} Torr. Once this flow has reached steady state (typically 1 minute), the QITMS is turned back on. During the injection phase ("injection" in Figure 5e), hydrogen carrier is rerouted through the PC chip and into the GC chip. The PC is then flash heated and the desorbed VOCs are flushed into the GC chip where chemical separation begins. For 10 to 20 minutes (depending on GC heater settings), eluted VOCs flow into the QITMS where they are ionized and detected ("chromatography" in Figure 5e). To enable nominal QITMS operating conditions during TGA the trap pressure is reduced by a factor of 20 by implementing a split-flow design in the TGA transfer line.

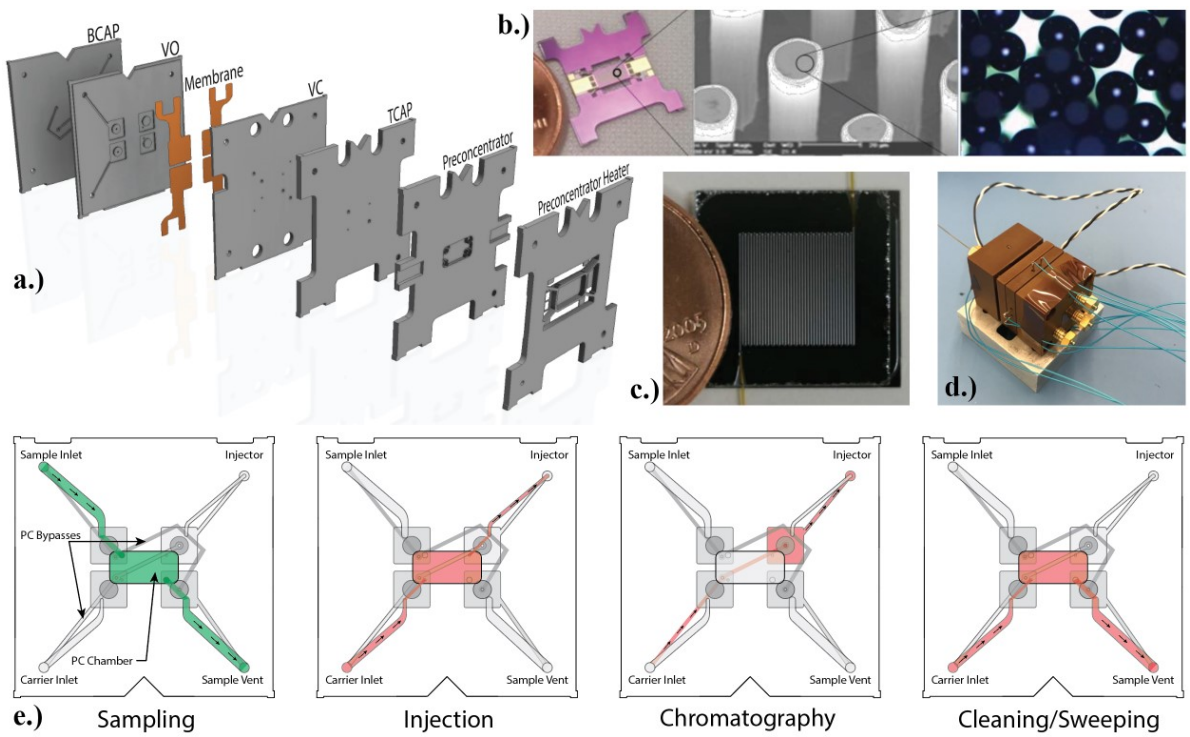

Figure 5. Overview of the MEMS PCGC components. *a.) Microfabricated layers that compose the microvalve (MV) and preconcentrator (PC) chips. b.) A zoomed in image showing the 250 nL PC chamber which is filled with Carboxen 1000 spheres used for chemical gain. c.) A picture of the inside of a GC microcolumn chip showing the compact serpentine column totaling 1 m in length. d.) The Vespel PCGC package which contains the PC, MV, and GC microchips in an extremely compact 1" x 1" x 2" configuration. The blue wires shown carry the electrical inputs used to drive the electrostatic membrane valves in the MV chip. Also shown are black and white wires to the PRT which monitors the heating of the GC chip. e.) Transparent overhead views of the multilayer MV and PC microchips for the different flow patterns used during a nominal TGA sequence. Green paths indicate the flow of sampled cabin-air while the red paths indicate the flow of H_2 carrier gas.*

In some cases, while chromatography occurs, a portion of the hydrogen flow is routed through the PC chip and into the sample inlet plumbing to backfill the volume with hydrogen to prevent lingering air from reaching the PCGC microchips (a combination of "chromatography" and "cleaning/sweeping" in Figure 5e). Once chromatography is completed, MDV2 is closed and the PC is heated once again while hydrogen is flowing through the PC chip as a means of post-cleaning ("cleaning/sweeping" in Figure 5e). After this post-cleaning step, the microvalves are unpowered and S.A.M. returns to MCA mode. Throughout this TGA sequence, the PCGC sample and carrier lines are heated to 50 ºC to prevent the adhesion of trace VOCs to the inner walls which might result in carryover between runs.

C. Overview of the S.A.M. Electronics

The S.A.M. electronics are designed to accommodate aggressive packaging requirements while meeting the demands to allow for QITMS operation with minimal power consumption, touchscreen control, WiFi communication, vacuum preservation fault detection, and full instrument autonomy. The compute element of S.A.M. is the open source Red Pitaya platform[19] which employs the Xilinx Zynq[20] and high speed waveform converters to perform instrument grade waveform synthesis and acquisition. The logic portion of the Zynq is programmed with the JPL FPGA firmware which controls the timing, rf generation, and pulse counting required for QITMS operation.

The major electronic subassemblies are the MS rigid flex assembly (MSRFA), the adjustable high voltage supply (AHVPS), the top and bottom endcap boards (ECBs), and the valve and heater control electronics (VHCE). The MSRFA (of which the Red Pitaya FPGA is a subcomponent) is responsible for generating the necessary voltage inputs to operate the QITMS. This input includes pulsed QIT electrode voltages, current for the tantalum filament, and amplified rf which is supplied to the SRL. The SRL design is a custom basket-weave of low-loss litz wire on a 3D printed polyetherimide (PEI) mandrel (2" x 5" x 5" in size).

The AHVPS generates the negative high voltage up to -2.8 kV used to bias the CEM for ion detection. An over-current protection circuit is included to prevent high current draws and repeated arcing in the case of overly high chamber pressures. The ECBs mount directly onto the custom titanium flanges of the QITMS vacuum chamber and serve as a wire routing and signal delivery solution to the internal QIT electrodes. Additionally, the bottom ECB houses a charge-sensitive preamplifier and discriminator (Amptek A121[21]) which converts CEM current signals into TTLs which are then counted by the Red Pitaya's fast pulse counter to form the S.A.M. mass spectra.

The VHCE is responsible for driving the various heaters, valves, and other sensors which populate the PCGC assembly. Also included on the VHCE board is a rad-tolerant ProAsic FPGA[22] which performs the fault detection and handling in the case of various anomalous events. Such events include (but are not limited to) over-pressurization of the QITMS chamber, loss of instrument power, loss of communication between FPGAs, and over temperature faults. In each case, the VHCE firmware safes the instrument by closing all Mindrum valves and shutting down QITMS operation to prevent risk of instrument damage.

The spectral recognition software used to determine the abundances of atmospheric major constituents and trace gases is called Random Walk (RW) and was developed in-house by S. Madzunkov and D. Nikolic. Briefly, the RW software is a linear regression algorithm which uses a basis set of known electron-impact fragmentation patterns provided by NIST to fit to experimental mass spectra. For each spectrum, the RW algorithm determines the vector of species counts which minimizes the error between the simulated and experimental spectra to ultimately produce partial pressure data for each species included in the basis. The RW algorithm is described in more detail elsewhere[23,24].

D. Network Communication with S.A.M. while onboard the ISS

During most of its lifecycle on the ISS, the S.A.M. payload will operate in a locker-configuration mounted in an EXPRESS Rack. The EXPRESS rack will provide a dedicated ethernet connection as well as other data interfaces to allow the S.A.M. team and other users to monitor and control the S.A.M. payload. There are two data links to ground provided by the EXPRESS rack which the S.A.M. payload will use: 1) a Ku-Band data link for telemetry monitoring and control via internet protocols and 2) an S-Band data link for payload health and status and critical commands. The S.A.M. TDU will be connected to the ISS on-board network through ethernet, which will allow data transfers at 10 Mbps or greater. The EXPRESS rack ethernet will provide data routing, time services via NTP, and telemetry flows either through S-Band (bridging to the 1553 bus) or directly through the KuIP services. Data will flow as TCP/IP for commands and important engineering telemetry, or as UDP for science telemetry. The data will be encapsulated as CCSDS packets and routed to the Payload Operations Center at Marshall Space Flight Center (MSFC). Error

Correction Code will not be used to protect the UDP telemetry packets against corruption due to the unlikelihood of significant impact given the volume and frequency of the telemetry data production.

Ground Controllers and the S.A.M. Team at JPL will have the primary responsibility of monitoring and controlling the payload from the JPL Earth Science Mission Operations Center (EOMOC). The Payload Operations Center at MSFC will also monitor the status of the S.A.M. payload using a dedicated health and status telemetry packet. The S.A.M. science telemetry data is transmitted to the ground via a Ku Band data link using the KuIP service (IP data over Ku Band) via the Tracking and Data Relay Satellite System (TDRSS) at the White Sands Complex in New Mexico. The data will be routed to the Huntsville Operations Support Center (HOSC) at MSFC, who will then route the data to JPL.

IV. S.A.M. Performance

To benchmark the S.A.M. performance throughout its maturation, successive development models were tested at the Environmental Control and Life Support System (ECLSS) facility at MSFC. At the ECLSS facility, the S.A.M. DMs were positioned in large chambers (called the E-Chamber and V-Chamber) which simulate ISS modules. Once sealed, the ECLSS facility infrastructure was used to create atmospheric dynamics of major constituents and trace gases. S.A.M. data taken during these dynamics were then compared to the reference data measured by internal ECLSS micro-GC sensor. This high-quality data was then used to inform future design decisions which ultimately led to the present form of the S.A.M. TDU.

E. S.A.M. Trace Gas Analysis

As of the writing of this manuscript, S.A.M. TGA testing has occurred once in the ECLSS V-Chamber at MSFC using the DM1 unit in May 2018, during which, perfluoropropane (PFP) was used as a test gas. To create trace levels of atmospheric PFP, pure PFP from a sample bag was pumped into the V-Chamber. Once stabilized, the S.A.M. DM1 began the nominal TGA sequence (previously described) using a sampling time of 25 minutes. A schematic overview of the TGA sequence and resultant chromatogram and mass spectrum for 7.5 PPM PFP is shown in Figure 6. In the top panel of Figure 6, the S.A.M. DM1 samples the V-Chamber atmosphere while remaining in MCA mode from t = 0 s until t = 1500 s. At this point the system is toggled into TGA mode followed by the PC injection occurring near t = 1600 s (indicated by a spike in detector counts due to electronic noise). The bottom left of Figure 6 panel shows the

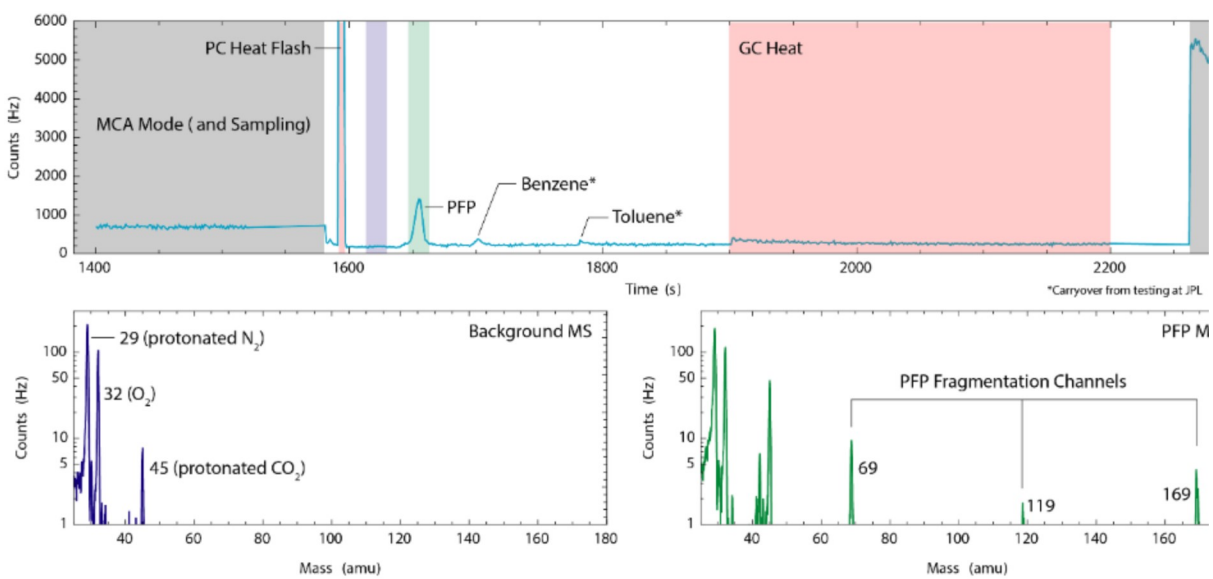

Figure 6. S.A.M. TGA Overview. *(Top) This chromatogram schematically shows a simplified TGA sequence during the injection of cabin-air with 7.5 PPM PFP, which includes sampling during MCA mode (first grey region), PC injection (first pink region), GC heat (second pink region), and the return to MCA mode (second grey region). (Bottom left) Mass spectrum taken at the beginning of the chromatography period (purple region) prior to the appearance of elution peaks. (Bottom right) Mass spectrum taken during the PFP elution peak.*

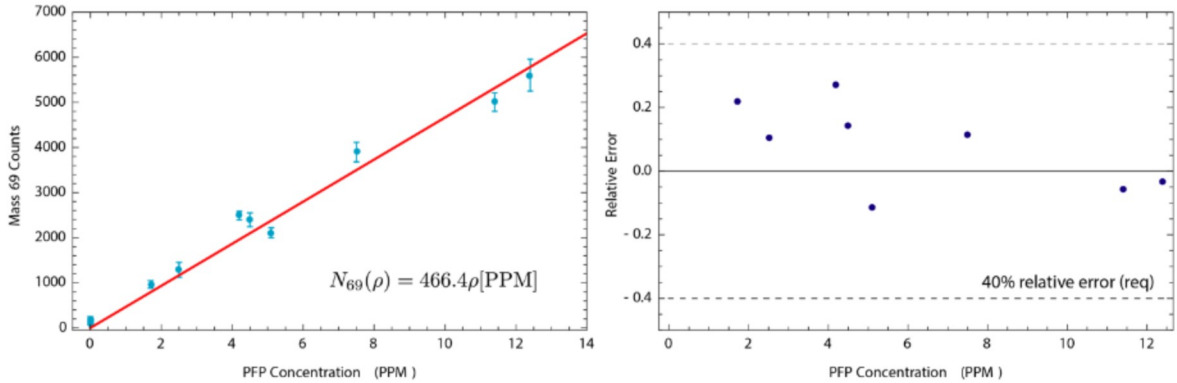

Figure 7. S.A.M. DM1 PFP Calibration. *(Left) Linear calibration (red) of measured PFP concentrations in the ECLSS V-Chamber to the mass-69 counts as recorded by the S.A.M. DM1 integrated over the entire PFP elution peak (cyan). Associated error bars represent Gaussian fit error to the elution peak. (Right) Error analysis reveals the counts-to-concentration calibration gives <40% relative error in terms of accuracy.*

background mass spectrum during TGA prior to the appearance of PFP, with major peaks at mass-29 (protonated nitrogen) and mass-32 (oxygen). At t = 1650 s, the PFP component appears in the chromatogram (top panel). The mass spectrum for PFP is shown in the bottom right panel of Figure 6 with major peaks at 69,119, and 169 amu. The PFP counts are integrated over the duration of the elution peak to determine the total PFP signal. During this analysis only the counts at mass-69 were included. This process was repeated eleven times for PFP concentrations ranging from 0 to 14 PPM.

The left panel of Figure 7 shows the cumulative mass-69 counts determined from the S.A.M. data plotted as a function of PFP concentration as measured by V-Chamber internal reference sensors. The cumulative mass-69 counts prove to be in good agreement with a linear relationship given by 466.4 counts per PPM PFP. The right panel of Figure 7 shows the relative error for each measurement residual as a function of PFP concentration confirming that a simple linear mapping of counts reported by S.A.M. is sufficient in determining the concentration of atmospheric PFP to within the required 40% error.

F. S.A.M. Major Constituent Analysis

To date, S.A.M. MCA testing has occurred twice in the ECLSS E-Chamber at MSFC – in May 2018 using the S.A.M. DM1 and in December 2018 using the S.A.M. DM2. Apart from numerous engineering and manufacturing improvements made between DM1 and DM2, the main difference regarding MCA between the two models was the MCA microleak used. In DM1, the MCA microleak dimensions were 1.5" x 1.3 µm ID which resulted in a 1.6 x 10^{-8} Torr L/s leak rate. In DM2, the MCA microleak dimensions were 3" x 3 µm ID which resulted in a 3.0 x 10^{-7} Torr L/s. Test data taken in the ECLSS E-Chamber showed that the DM1 MCA microleak was slightly too small, leading to a count rate that prohibited the DM1 from reaching its precision requirements in the allotted integration time. On the other hand, ECLSS test data showed that the DM2 microleak was slightly too large, leading to large amounts of detector saturation for nominal QITMS operating parameters. As a result, the S.A.M. TDU is equipped with a 5.0 x 10^{-8} Torr L/s microleak (1.5" x 2.0 µm ID), which satisfies our precision requirements without the onset of detector saturation. As of the writing of this manuscript, the S.A.M. TDU has yet to be tested at the ECLSS facility. Consequently, representative MCA data for oxygen, nitrogen, and carbon dioxide taken using the S.A.M. DM1 will be presented here. Since the DM1 was not exposed to methane atmospheres, methane data taken with DM2 will be shown.

The S.A.M. DM1 response to changes in atmospheric oxygen in the ECLSS E-Chamber is shown in Figure 8 alongside internal reference sensor data. Each S.A.M. data point consists of 20 s of integration (equivalent to 6 s with the TDU MCA leak rate) compared to 2 to 3 minutes of integration for each ECLSS sensor data point. A histogram of the S.A.M. measurement residuals is shown in the right panel of Figure 8 which clearly exhibits the Gaussian-like shape indicative of uncorrelated Poissonian events with large *N*. The absolute 1-sigma error associated with this distribution is ±0.2% (±1.5 Torr) for concentrations between 17.7% and 22.6% (134 to 172 Torr). This error analysis assumes no error in the reference measurement and therefore represents a conservative estimate.

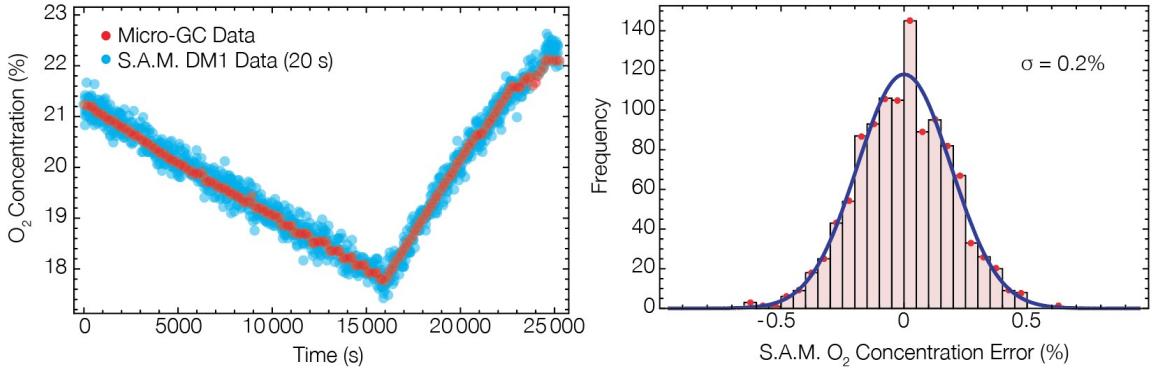

Figure 8: O_2 monitoring using S.A.M. DM1. *(Left) The S.A.M. DM1 (cyan) and ECLSS micro-GC (red) responses to the changing O_2 concentration (18-22%) in the E-Chamber. Each S.A.M DM1 data point corresponds to a 20 s integration whereas each ECLSS micro-GC data point corresponds to 2-3 minutes of sampling. Because the DM1 MCA leak is roughly 3x smaller than the TDU MCA leak, this data is analogous to ~6 s averages using the TDU. (Right) Analysis of the DM1 O_2 measurement error gives an absolute precision of ±0.2% (±1.5 Torr).*

The S.A.M. DM1 responses to changes in atmospheric nitrogen and carbon dioxide are shown in Figure 9 again alongside internal reference sensor data. Likewise, the associated measurement errors are indicated by the corresponding residual histograms. The absolute 1-sigma error for the nitrogen measurement is ±0.2% (±1.5 Torr) for concentrations between 74.7% and 95.6% (567 to 727 Torr). The absolute 1-sigma error for the carbon dioxide measurement is ±0.08% (±0.6 Torr) for concentrations between 0.05% and 0.97% (0.4 to 7.3 Torr).

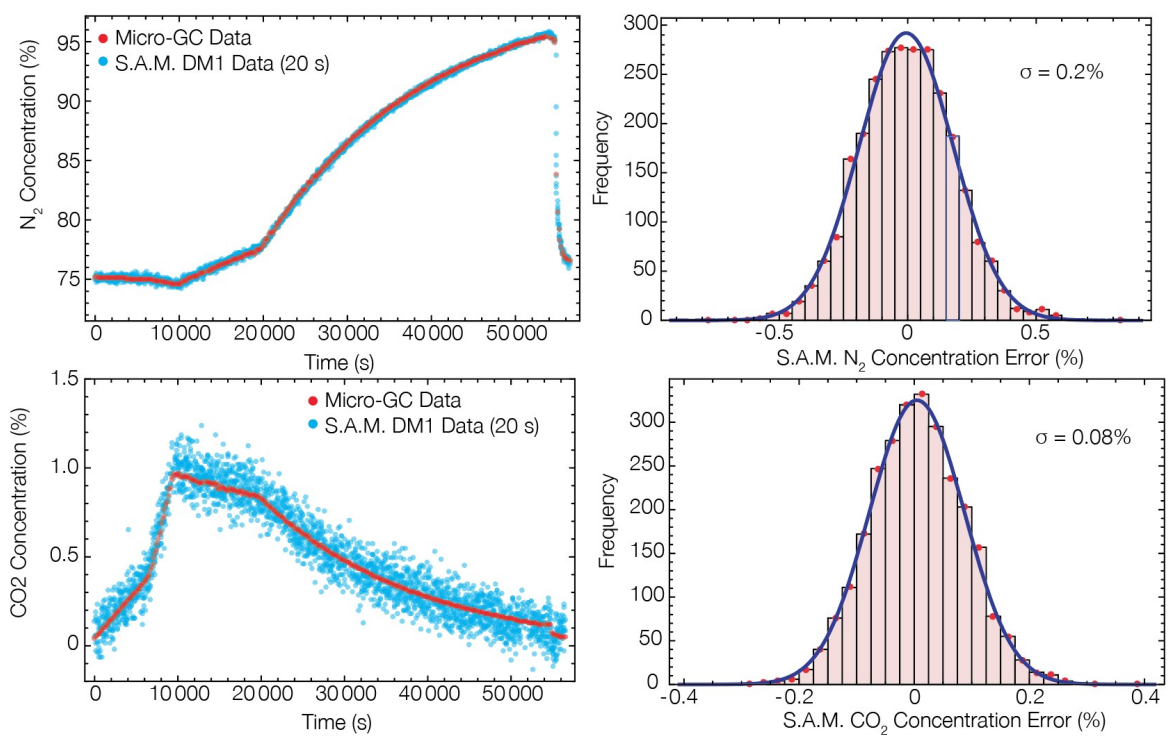

Figure 9. N_2 (top) and CO_2 (bottom) monitoring using the S.A.M. DM1. *(Left panels) The S.A.M. DM1 (cyan) and ECLSS micro-GC (red) responses to the changing N_2 concentration (75-96%) and CO_2 concentration (0.05-1.0%) in the E-Chamber.. (Right panels) Analyses of the DM1 N_2 and CO_2 measurement errors give absolute precisions of ±0.2% (±1.5 Torr) and ±0.08% (±0.6 Torr).*

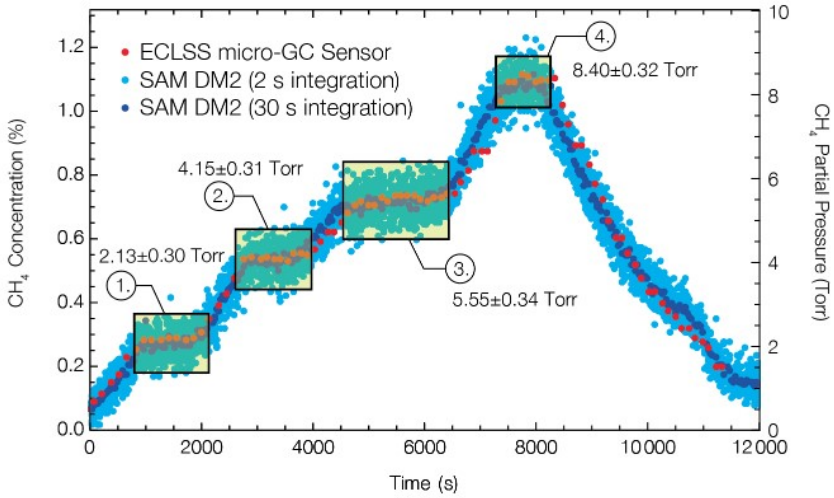

Figure 11. CH_4 monitoring using S.A.M. DM2. *The S.A.M. DM2 data for CH_4 is shown for 2 s (cyan) and 30 s (dark blue) integration times alongside the ECLSS micro-GC data (red), which has a 2-3 minute measurement time. The CH_4 levels are increased from 0 to 1.1%. The associated absolute measurement precision, analyzed at the four plateaus (yellow), is shown to be relatively constant at 0.04% (±0.3 Torr) using 2 s integration times.*

To benchmark its response to changes in atmospheric methane, the S.A.M. DM2 was positioned in the ECLSS V-Chamber and exposed to increasing levels of methane. Figure 11 shows the S.A.M. DM2 data (2 s and 30 s integration times) alongside internal reference sensor data (2 to 3 min integration times). At various partial pressures, the increase in methane was stopped for short periods of time to determine the DM2 measurement error (indicated by the yellow shaded regions). The corresponding residual histograms are also shown and indicate an absolute 1-sigma error of approximately ±0.04% (±0.3 Torr) for the entire range between 0 and 1.1% (0 to 8.4 Torr) using 2 s integration times.

Despite not having benchmarked S.A.M. TDU performance in the ECLSS facility at MSFC, lab testing at JPL using the planned TDU microleak has been performed using static atmospheric abundances. Figure 10 shows a representative mass spectrum alongside the residual histograms which have absolute 1-sigma errors of ±0.07% (±0.5 Torr), ±0.07% (±0.5 Torr), and ±0.01% (±0.1 Torr) for nitrogen, oxygen, and carbon dioxide respectively. The reporting requirement for methane could not be evaluated (due to the lack of methane in our atmospheric air sample),

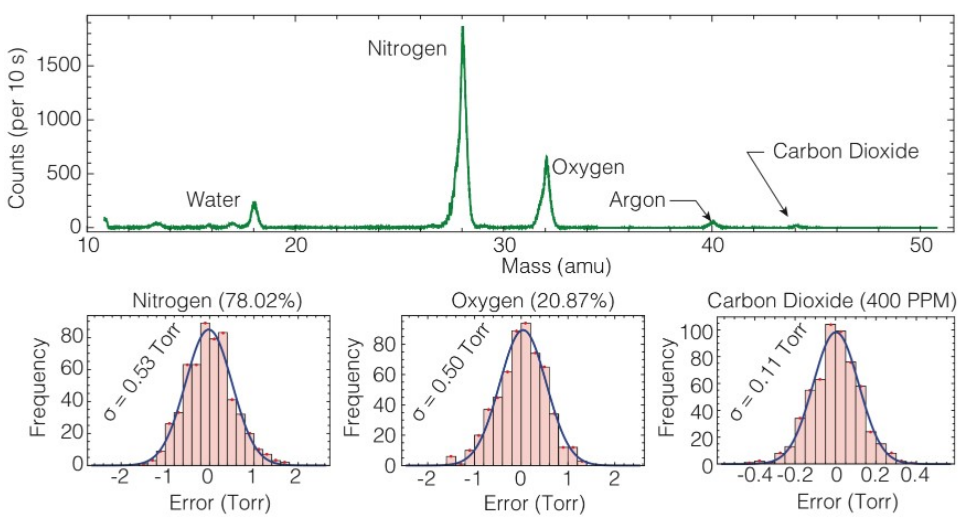

Figure 10. Current S.A.M. TDU MCA Performance. *(Top) Representative mass spectrum of the static S.A.M. lab atmosphere at JPL produced using the planned TDU MCA microleak. (Bottom) Analyses of the N_2, O_2, and CO_2 measurement errors using 10 s integration give precisions of ±0.07% (±0.5 Torr), ±0.07% (±0.5 Torr), and ±0.01% (±0.1 Torr), respectively. CH_4 was not measured here.*

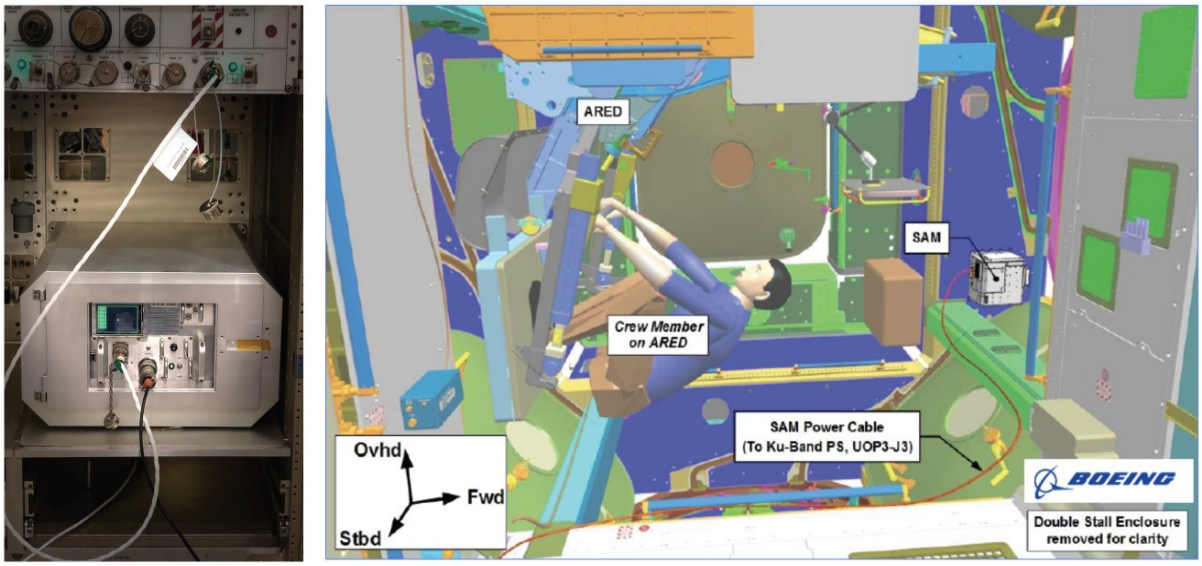

Figure 12. S.A.M. Deployment on the ISS. *(Left) S.A.M. DM2 in its locker-configuration mounted in an EXPRESS rack for ground testing at the Space Systems integration and Test Facility at MSFC. (Right) Mockup, generated by Boeing, of the S.A.M. TDU in its aisle-deployed configuration in the tranquility Node 3 on the ISS. This location will enable S.A.M. to monitor trace gases being emitted from astronauts engaging in strength training using the Advanced Resistive Exercise Device (ARED).*

however based on noise levels at mass-15 we expect a 1-sigma error <0.5 Torr. A summary of the current capabilities of the different S.A.M. models is given in Table 1.

V. Plan Forward

The S.A.M. TDU is scheduled for launch in mid-2019 on the SpaceX-18 ISS resupply mission aboard its Dragon capsule (a pressurized cargo vehicle). After docking with the ISS, the S.A.M. payload (which includes the TDU and its stowage locker) will be installed by the astronauts into the ISS EXPRESS rack as shown in the left panel of Figure 12. On-station, the S.A.M. TDU will not require crew member operation after installation, but will enable crew-member-initiated actions via the HIM.

During the first few weeks on-station, the S.A.M. TDU will perform daily 10 to 20 minute TGA runs in order to gauge the instrument's repeatability and diagnose the degree of carryover between runs. As the S.A.M. TDU transitions further into its life cycle, daily TGA runs will be relaxed to weekly TGA runs with the option to perform on-demand TGA runs in the event of anomalous odors or occurrences on-station. Additionally, planned aisle-deployments to US Lab locations in Nodes 1, 2 , and 3 will allow the S.A.M. TDU to perform TGA runs in the vicinity of astronaut activities in order to gain insight into the source and quantity of different VOCs in the cabin air. The right panel of Figure 12 shows a mockup of the S.A.M. TDU aisle-deployed in the Tranquility Node 3 of the ISS which contains the Advanced Resistive Exercise Device (ARED). When not performing TGA, the S.A.M. TDU will be in MCA mode issuing updated major constituents reports every 2 s.

While on-station, mass spectrometry data as well as instrument telemetry regarding health and status of the instrument will constantly be routed through the HOSC to the S.A.M. operation team at JPL's EOMOC. While the S.A.M. TDU is fully autonomous and does not require data processing for issuing reports of major constituents and trace gases, JPL scientists will have the ability closely analyze the data for the occurrence of interesting or anomalous findings.

Acknowledgments

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