JSC TOXICOLOGY AND ENVIRONMENTAL CHEMISTRY GROUP

E. Spencer Williams, PhD, DABT
Toxicology and Environmental Chemistry
NASA JSC/SK4
Houston, TX 77058

Memorandum Number
TOX-SW-2019-04

Voice: (281) 483-8921
Fax: (281) 483-3058
edward.s.williams@nasa.gov

DATE: May 1, 2019

SUBJECT: Toxicological Assessment of ISS Air and Water Quality: June 3, 2018 – October 4, 2018 (Increment 56), Including HTV-7 Ingress

SUMMARY: Based on these data, air quality was acceptable on ISS for this period and potable water remains acceptable for crew consumption.

AIR QUALITY

Six archive air samples were collected in mini grab sample containers (mGSCs) on ISS during Increment 56. At the request of the crew, a contingency sample was collected in Node 1 on July 2, 2018 due to an ongoing trash odor. Routine samples were collected on July 10 and August 21, 2018. One additional sample was collected during first ingress operations in HTV-7 (September 27, 2018). Samples collected in July were returned on SpX-15 and samples from August and September were returned on SpX-16. Due to procedural issues, no mGSC sample was collected at SpX-15 ingress. A summary of analytical results from the samples is provided in Table 1. A pair of passive-diffusion formaldehyde badges were deployed in the Lab and Service Module (SM) on July 10, 2018. However, they were not retrieved until 43 days later. Another set was deployed on August 21, 2018 and retrieved on August 23rd. Aside from the longer-than-expected deployment period for badges in July, analysis of these samples and the associated controls revealed potential issues with the lot of formaldehyde badges delivered on OA-9. Due to concerns about the performance of the badges, data for formaldehyde are not reported for Increment 56.

Table 1. Analytical summary of ISS air analyses (Increment 56)

Return Flight	Sample Location	Sample Date	Freon 218 (mg/m3)	Alcohols[a] (mg/m3)	T-Value[b] (units)	Formaldehyde (µg/m3)
SpaceX-15	Node 1	7/2/2018	150	16	0.6	---
SpaceX-15	LAB	7/10/2018	140	12	0.3	---
SpaceX-15	Columbus	7/10/2018	150	13	0.3	---
SpaceX-16	LAB	8/21/2018	114	9.6	0.3	---
SpaceX-16	SM	8/21/2018	115	16	0.4	---
SpaceX-16	HTV-7 ingress	9/27/2018	3.7	3.8	1.2 (0.9)	---
Guideline			---	*<5*	*<1*[c]	*<120*

[a]Includes acetone
[b]Sum of the ratios of the measured concentration and the corresponding 180-day SMAC for each compound, excluding CO_2; parentheses indicate value based on 7-day SMACs and applicable to first ingress
[c]T-value <1 used to evaluate routine monthly sampling; <3 used to evaluate first ingress

Data tables containing measured concentrations and corresponding T-values based on appropriate Spacecraft Maximum Allowable Concentrations (SMACs) for compounds present at levels above the laboratory reporting limit are attached to this report. Complete data tables, which include compounds assessed but not detected, are available upon request. The mean relative recoveries of the three surrogate standards from the mGSC samples returned on SpX-15 and -16 were within acceptable limits.

The Air Quality Monitors (AQMs) automatically collect data every 73 hours, which results in 2-3 sampling sessions per unit per week. Monthly average concentrations as well as the increment average concentrations for compounds measured on the AQMs are presented in Table 2.

Table 2. Average monthly concentrations (mg/m^3) of AQM target compounds

Compound	June Average	July Average	August Average	September Average	October Average	Increment Average
2-Propanol	0.2	0.2	0.1	TRACE	0.1	0.2
Acetone	0.2	0.2	0.2	0.2	0.1	0.2
Acrolein	ND	ND	ND	ND	ND	ND
Benzene	ND	ND	ND	ND	ND	ND
1,2-Dichloroethane	ND	ND	ND	ND	ND	ND
Decamethylcyclopentasiloxane#	0.2	0.2	0.2	0.2	0.2	0.2
Hexanal	ND	ND	ND	ND	ND	ND
Hexane	ND	ND	ND	ND	ND	ND
m,p-Xylenes#	ND	ND	ND	ND	ND	ND
Methanol	0.2	0.2	0.2	0.2	0.2	0.2
o-Xylene#	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Octamethylcylcotetrasiloxane#	TRACE	TRACE	TRACE	TRACE	TRACE	TRACE
Toluene#	ND	ND	ND	ND	ND	ND
2-Butanone	ND	ND	ND	ND	ND	ND
Acetaldehyde	0.3	0.4	0.4	0.3	0.3	0.4
Dichloromethane	ND	ND	ND	ND	ND	ND
Ethanol	1.7	3.0	6.6	5.7	4.8	4.4
Ethyl Acetate	0.1	0.1	0.1	0.1	0.04	0.1
Hexamethycyclotrisiloxane#	0.04	TRACE	0.1	0.1	0.1	0.1
n-Butanol	TRACE	TRACE	0.1	0.1	0.1	0.1
Trimethylsilanol	TRACE	TRACE	0.1	0.1	0.1	0.1

Obtained from prime unit
ND: Not detected; <MDL (Minimum Detection Limit)
TRACE= >MDL, <MQL (Minimum Quantification Limit)
Note: Increment 56 included 4 days in October.

Toxicological Evaluation of ISS Air Quality

Routine air quality monitoring is performed in-flight using the AQMs. Archive air samples (mGSCs and formaldehyde badges) are collected during each increment and returned for analysis in the Toxicology and Environmental Chemistry (TEC) Air Quality Laboratory. Data from the ground analyses complement the in-flight data and provide a more complete understanding of air quality on the ISS. The routine archive samples for this increment that returned on SpX-15 and -16 confirmed air quality was acceptable. **All measured values for routine samples (mGSC and AQM) met 180-d T-value guideline criteria (T < 1), indicating no concern for crew health.** The average, rounded T-value calculated from the Increment 56 mGSC samples was 0.3 (Figure 1), similar to Increments 53-55 and remains well below levels of concern. T-values for specific health effects were calculated using data collected on the AQMs (Figure 2). The T-

values calculated from GSC results and AQM data are in reasonable agreement given the differences between the analytical techniques and the number of target compounds used in the calculation.

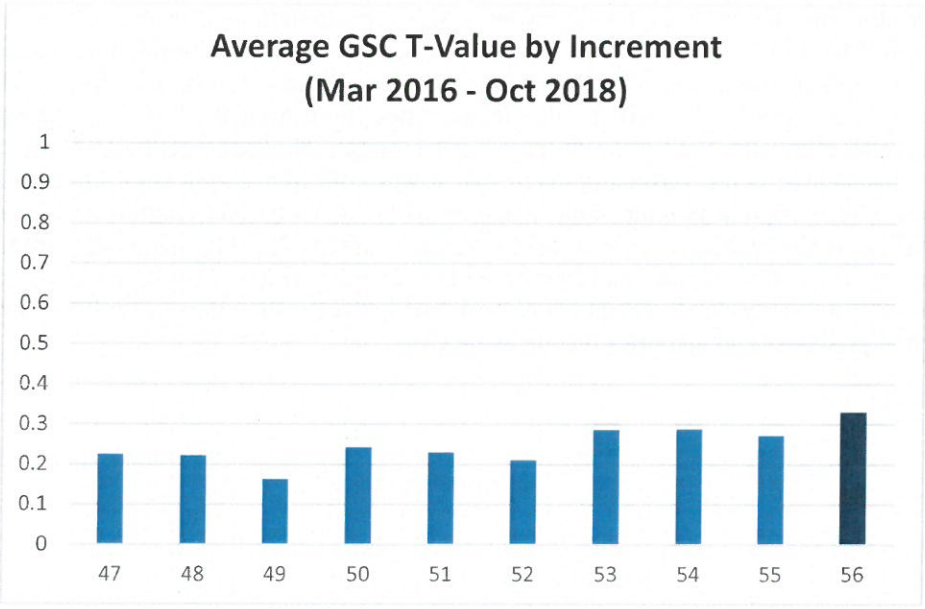

Figure 1. T-values Derived from Nominal mGSCs for Increments 47- 56

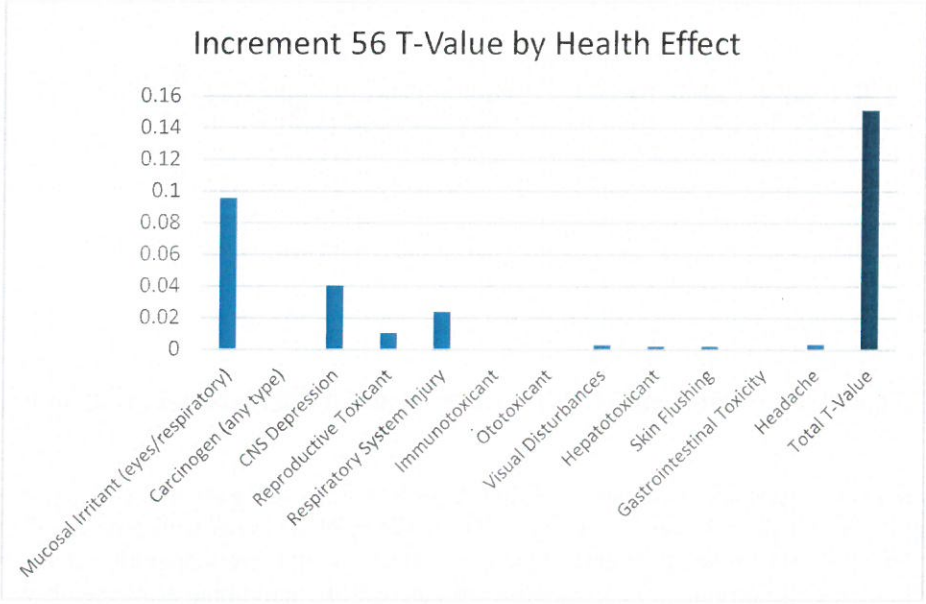

Figure 2. AQM-Derived T-Values by Health Effect for Increment 56

Generally, the reported concentrations for the compounds detected during Increment 56 are similar to levels detected during recent increments. This includes atmospheric concentrations of siloxanes (i.e., TMS, OMCTS, and HMCTS). The slight increase in T-value compared to Increment 55 appears to be mostly

attributable to levels of acetaldehyde. T-values for this compound were ~0.12 in Inc 55 vs. 0.015 (average) in Increment 56.

Three of the nominal mGSC samples contained a CO_2 concentration at or below the increment limit documented in Chit 14468, which requests that the 24 hour average concentration not exceed 3.0 mmHg (7100 mg/m^3) on the US segment. The contingency sample collected in Node 1 on July 2, 2018 was above the Chit limit (8200 mg/m^3; 3.5 mmHg). The sample collected on August 21, 2018 in the Russian Service Module was also above the limit (12,100 mg/m^3; 5.4 mmHg). The fact that the CO_2 concentration was elevated in this sample is not surprising given that it was collected during split atmosphere operations. While mGSC CO_2 sampling provides only a snap-shot of the CO_2 concentration, the major constituent analyzer (MCA) routinely monitors CO_2 levels in the US segment. For this reason, data from the MCA are better suited for evaluation of short and long-term trends in CO_2 (Figure 3). Concentrations measured by the MCA fluctuate as a result of multiple factors including the number of crew on ISS, current scrubbing capability, and processes and activities that generate CO_2.

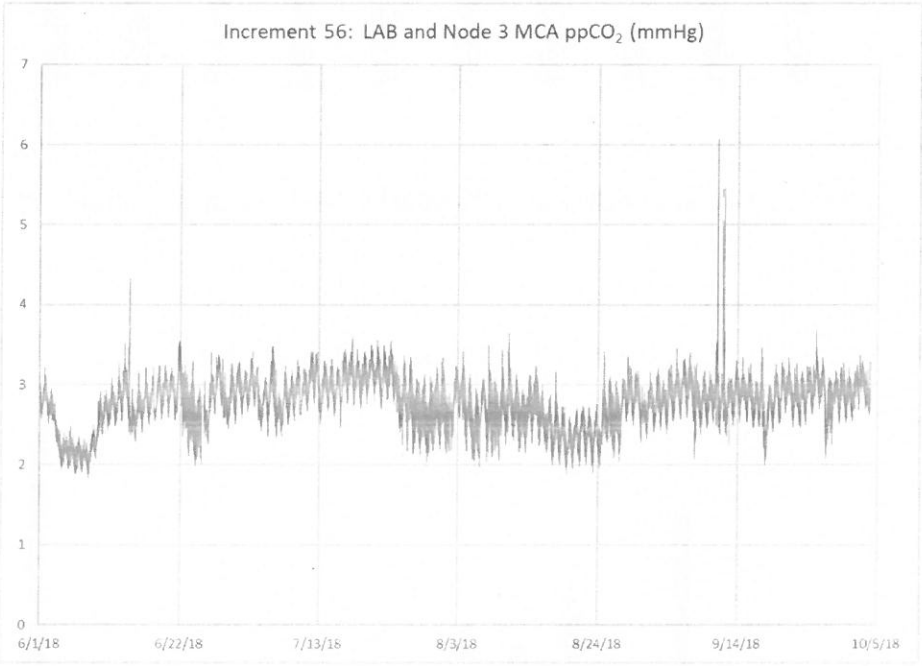

Figure 3. Environmental CO_2 Concentrations on ISS Increment 56 in mmHg

Data for most of the increment were obtained from the MCA in the US Lab. Some data in September were obtained from the MCA in Node 3. Overall, CO_2 concentrations were well-controlled throughout the increment. The drop in CO_2 levels in early June is consistent with 3- crew operations (departure of Soyuz on June 3rd), and the rise on June 6th corresponds with arrival of 3 additional crew members. An excursion in CO_2 above 4 mmHg was observed during an EVA conducted on June 14th. Split atmosphere operations were conducted from August 16-24, 2018. During this period, the CO_2 concentration in the Russian Segment reached 6.7 mmHg (August 20th according to BME logs). As noted above, the SM mGSC sample collected on August 21st showed a concentration of 12100 mg/m^3 (6722 ppm, ~5.4 mmHg). Intermodule ventilation was temporarily re-established and the Node 3 carbon dioxide removal assembly (CDRA) was

activated to help reduce the concentration. MetOx regeneration conducted on September 10th and 11th coincides with a brief but notable increase in CO_2.

An air selector valve on the Lab CDRA failed on June 21st, so the Node 3 CDRA and amine swingbed were activated to manage CO_2 levels. The failed valve was replaced on June 25th. To address rising CO_2 levels in mid-July, a Russian LiOH cartridge was activated on July 23rd, and the amine swingbed was activated on July 24th. CO_2 levels decreased over the following weeks.

As previously noted, CO_2 was measured at 12,100 mg/m^3 (5.4 mmHg) in the August 21 SM mGSC, which is lower than the levels measured on the previous day (6.67 mmHg on August 20th). In addition to CO_2, concentrations of several analytes were markedly higher in the Russian SM during split atmosphere operations. Total alcohols plus acetone were 16 mg/m^3 in the SM, compared with 9.6 mg/m^3 in the US Lab at the same sampling time. Ultimately, the T-value for this sample was modestly higher (0.38) compared to the concurrent sample in the US Lab (0.30).

Alcohol values in all routine archive samples continued to exceed the ECLS guideline of <5 mg/m^3, which is intended to protect the U.S. Water Recovery System (WRS) from overloading. These levels are primarily due to ethanol in the ISS atmosphere. AQM results for ethanol rose in Increment 56 (average = 4.4 mg/m^3) compared to Increment 55 (average = 3.8 mg/m^3), including a peak of 6.6 mg/m^3 in August. Ethanol levels observed in mGSC samples collected during Increment 56 were also modestly higher (8.3 – 15 mg/m^3) than those observed during Increment 55 (7.6 – 11 mg/m^3). The GSC sample from May (Increment 55) contained a total alcohols (plus acetone) level of 17 mg/m^3. Results from July and August were slightly lower (9.6-16 mg/m^3), with the highest result coming from the Russian segment during split atmosphere operations. The increase in total alcohols at the end of Increment 55 and sustained levels during Increment 56 warrants additional scrutiny of the trend in the future.

Octafluoropropane (Freon 218) levels continued to decrease throughout the increment following the release during Increment 53. This concentration is more than two orders of magnitude below the 180-d SMAC value (85,000 mg/m^3) and does not constitute a toxicological risk.

As mentioned above, there were several issues with the passive formaldehyde badges in Increment 56. Badges were deployed on July 10, 2018 but not retrieved for 43 days. Another set was nominally deployed on August 21, 2018 and retrieved on August 23rd. These badges were returned on Soyuz 55. The badges were analyzed, but the results and the calculated recoveries for control badges raised concerns about the validity of the data. Due to these concerns, no formaldehyde data is being reported for Increment 56. JSC TEC is investigating the issue and will be evaluating alternative approaches to the assessment of formaldehyde in ISS air.

Node 1 Contingency Sample

On June 5th, the crew reported odors in Node 1 near the Cygnus vehicle (OA-9) and asked for permission to close the hatch, as they often eat in the adjoining space. They were instructed to use fans to redirect the airflow. A contingency air sample was collected on July 2nd. The sample contained 0.12 mg/m^3 carbon disulfide, a common air pollutant associated with solid waste odors. Methane was also slightly higher in this sample than samples taken on July 10th in the Lab and Columbus (8200 vs 7100 mg/m^3). The total T-value for this sample was 0.56, well below levels of concern for crew health. However, the measured carbon disulfide levels could easily be associated with the crew odor reports, resulting in potentially degraded habitability during this timeframe. These findings should inform operational considerations in the future. OA-9 unberthed on July 15th and was deorbited on July 30th.

HTV-7 Ingress

A GSC sample was collected upon ingress into HTV-7 on September 27, 2018 at 19:50 GMT, approximately five minutes after hatch opening. **The measured T value (excluding CO_2) of 0.9 was well below levels of concern for crew health.** No background concentration of Freon 218 (octafluoropropane), a marker for ISS air dilution of first entry samples, was available near the time of first ingress sampling for comparison; however, the concentration of Freon 218 in the ingress sample was 3.7 mg/m^3, markedly lower than levels detected in the US Lab and Russian SM on August 21, 2018 (114 and 115 mg/m^3 respectively), which suggests limited mixing. Carbon dioxide in the ingress sample was 1500 mg/m^3 (830 ppm; 0.6 mmHg), which also suggests limited mixing. The primary contributors to the calculated T-value were trimethylsilanol (2.4 mg/m^3) and carbon disulfide (0.14 mg/m^3).

On August 29, 2018, a leak was detected due to a drop in pressure on ISS. After an extensive search, a small hole was found in a Soyuz vehicle and was successfully patched. This leak does not appear to have had a measurable effect on the air quality on ISS.

WATER QUALITY

Six archive water samples were collected from the US segment during Increment 56 and returned on Soyuz 54. Samples of wastewater and condensate were collected on July 10, 2018. Samples of product water from the Water Processor Assembly (WPA) were collected from the potable bus in the US Lab on July 26, 2018 and a sample of hot water was collected from the Potable Water Dispenser (PWD) on September 10, 2018. A sample of condensate from the Columbus module was also collected during Increment 56 (July 17, 2018) and returned on SpX-15. The sample of Columbus condensate was collected as part of an on-going investigation into the source of dimethylsilanediol (DMSD) in the ISS atmosphere. Complete data tables with results for all measured parameters can be found in reports 2018-TEC-WQ-006 (SpX-15) and 2018-TEC-WQ-007 (Soyuz 54). A summary of select analytical results from the Increment 56 samples is provided in Table 3. Expanded summary tables containing organic carbon recoveries and results for all analytes present at concentrations above reporting limits are included as attachments to this report.

Table 3. Analytical Summary of ISS Water Analyses (Increment 56)

Return Mission	Sample Location	Sample Date	TOC (mg/L)	DMSD (mg/L)	Methyl Sulfone (mg/L)	Conductivity (mS/cm)	Total Iodine (mg/L)
Soyuz 54	Wastewater	7/10/2018	27.7	25,000	0.21	173	NA
Soyuz 54	Condensate	7/10/2018	134	38,000	0.19	240	NA
SpaceX-15	Condensate	7/17/2018	187	60,000	0.23	350	NA
Soyuz 54	US Lab Potable Bus (pre-flush)	7/26/2018	0.86	< 1000	NA	6	3.78
Soyuz 54	US Lab Potable Bus (post-flush)	7/26/2018	1.17	2700	NA	2	1.83
Soyuz 54	WPD PWD Hot	9/10/2018	0.42	< 1000	0.15	2	< 0.05

NA: not analyzed

Toxicological Evaluation of ISS Water Quality: Routine water quality monitoring is performed in-flight using the total organic carbon analyzer (TOCA). Results from these analyses provide a general indication of overall water quality. Archive water samples are collected during each increment and returned for comprehensive analysis in ground laboratories. Data from the ground analyses complement the in-flight data and provide a more complete understanding of water quality on the ISS.

Potable Water

Concentrations of all chemicals detected in the potable water samples met the requirements listed in SSP 41000, *System Specification for the International Space Station* and JSC 63414, Spacecraft Water Exposure Guidelines (SWEGs). Total organic carbon (TOC) concentrations from in-flight (PWD TOC and WPA TOC) and ground analyses (Archive TOC) performed between October 2016 and October 2018 are shown in Figure 4. The TOC concentration in the potable sample (0.42 mg/L) was lower than the concentrations measured in the sample returned on Soyuz 53 (1.02 mg/L hot and 1.05 mg/L ambient). This decrease was the result of a new ion exchange (IX) bed being installed in the WPA in August 2018. The TOC concentration in the potable sample was well below both the U.S. Segment Specification (3000 µg/L) and the 100-day SWEG (5000 µg/L). Methyl sulfone, often a minor contributor to the TOC, was detected in the PWD hot sample at a level lower than observed in Increment 54 (0.31 mg/L) and similar to Increment 55 (0.13 mg/L), but still higher than the historical average for hot water (0.08 mg/L). Although the concentration of this compound trended upward over several increments, levels have stabilized and are still well below the SWEG of 1,500 mg/L. Silicon levels in the potable samples dropped markedly from Increment 55 to 56. This decrease can be attributed to the installation of the new IX bed as DMSD (primary compound responsible for silicon in potable water) is retained on new beds. TOCA continued to under-report TOC results compared to the archival samples during the Increment even though results from TOCA calibration checks meet their specifications. Continued monitoring of TOCA performance should continue to assess whether maintenance is needed.

Iodine is a biocide used on the US segment. It is added to the water produced by the WPA, but removed prior to crew consumption to avoid potential thyroid dysfunction. The total iodine level in the potable sample collected from the PWD on September 10, 2018 was below the reporting limit (0.05 mg/L), indicating effective removal of iodine. For information regarding microbial analyses performed on the potable sample, please see the Increment 56 post-flight report issued by the JSC Environmental Microbiology Laboratory

Product Water

The U.S. Water Recovery System (WRS) was originally installed in the U.S. Lab and connected to the Lab potable bus. It remained in that location until February 2010 when it was relocated to Node 3. Following the WRS move, the Lab potable bus remained stagnant filled with WPA product water. With the planned installation of the Life Support Rack in the U.S. Lab (which will be connected to the potable bus), the potable bus in the U.S. Lab was flushed to remove the stagnant water. Samples of the water in the bus were collected before and after the flush to check for potential contamination in the bus.

The TOC concentrations in the product water samples 0.86 mg/L (pre-flush) and 1.17 mg/L (post flush). The primary contributor to TOC in the post-flush potable sample was DMSD (2.7 mg/L). Virtually no organic contaminants were detected in the pre-flush sample. The level of nickel in the pre-flush sample (1.8 mg/L) was consistent with expectations for stagnant water in contact with stainless steel for an extended time. The concentration dropped down to 0.05 mg/L in the post-flush sample, which indicates the stagnant water was successfully purged from the line.

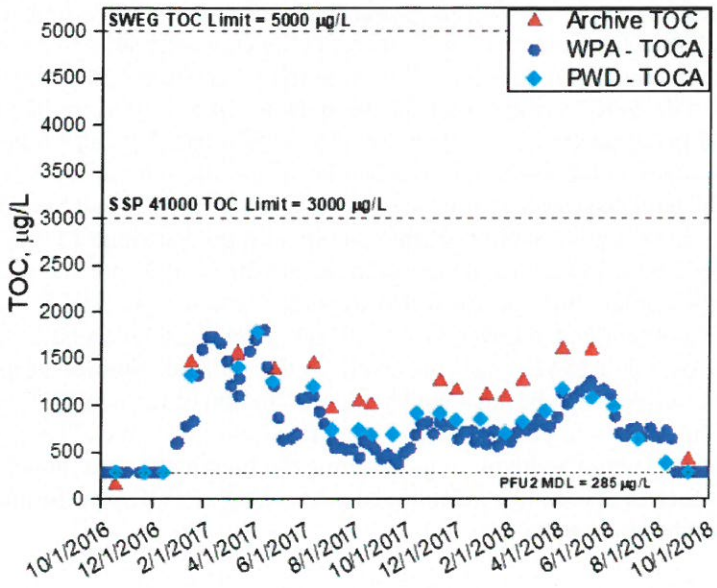

Figure 4. Total Organic Carbon (TOC) trending in US Potable Water

The iodine concentration in the pre- and post-flush samples collected from the Potable Bus were 3.78 and 1.83 mg/L, respectively. While this water was not intended for consumption, the iodine levels were below the permissible limit of 6 mg/L. The primary form of iodine in the pre-flush sample was iodide, which is non-biocidal. This is consistent with expectations as it is known that molecular iodine (I_2, biocidal form) is reduced to iodide when in contact with stainless steel. The post-flush sample contained 1.34 mg/L of active biocidal iodine, which confirms that the flush was effective. For information regarding microbial analyses performed on the product water samples, please see the Increment 56 post-flight report issued by the JSC Environmental Microbiology Laboratory.

U. S. Condensate

The condensate sample collected on July 10, 2018 contained a TOC level of 134 mg/L, which is below the historical average (162 mg/L). These results are consistent with AQM results indicating that ISS air quality was well managed for the Increment. Non-metal compounds detected at levels greater than 1 mg/L included DMSD (38 mg/L), ammonium (31.8 mg/L), silicon (12.6 mg/L), benzoic acid (2.6 mg/L), benzyl alcohol (21.6 mg/L), 2-(2-Butoxyethoxy)ethanol (1.2 mg/L), 2-Phenoxyethanol (1.9 mg/L), acetone (3.8 mg/L), ethanol (101 mg/L), isopropanol (1.2 mg/L), methanol (8.5 mg/L), propylene glycol (12 mg/L), ethylene glycol (2.8 mg/L), and acetate (41.2 mg/L). Zinc (3.4 mg/L), nickel (0.17 mg/L), and traces of other metals were also present in this sample.

U. S. Wastewater

The wastewater sample collected on July 10, 2018 contained a TOC level of 27.7 mg/L, which was markedly lower than the wastewater sample from Increment 55 and lower than the historical average of 44.6 mg/L. Ethanol was not detected in this wastewater sample. The DMSD concentration was 25 mg/L, and acetone was detected at 9 µg/L. Non-metal compounds detected at levels greater than 1 mg/L included methanol (3.8 mg/L) ammonium (22.4 mg/L) and silicon (8.5 mg/L). Of metals analyzed, only zinc (0.98

mg/L) was detected above 0.1 mg/L. Traces of boron and nickel were also present. The ammonia detected in the wastewater sample (22.4 mg/L) was well above the historical average (17.7 mg/L).

Columbus Condensate
The TOC concentration in Columbus condensate sample (collected on July 17, 2018) was 187 mg/L. Organic compounds present at concentrations greater than 1 mg/L include acetate (160 mg/L), DMSD (60 mg/L), benzyl alcohol (25 mg/L), propylene glycol (15 mg/L), acetaldehyde (15 mg/L), ethylene glycol (6.8 mg/L), 2-propanol (4.2 mg/L), caprolactam (2.5 mg/L), benzoic acid(2.3 mg/L), 2-(2-butoxyethoxy)ethanol (1.8 mg/L), diethylphthalate (1.5 mg/L), N,N-dimethylacetamide (1.4 mg/L), nonanoic acid (1.4 mg/L), acetone (1.1 mg/L), and hexanoic acid (1.1 mg/L). Silicon was present at a concentration of 29.6 mg/L, most of which can be attributed to the presence of DMSD. Calcium and potassium were found at detectable levels, and low levels of nickel and zinc were also present in the sample.

All of the compounds detected in the condensate and wastewater samples were effectively removed by the WRS, as evidenced by the low or undetectable levels in the potable sample.

E. Spencer Williams, Ph.D., DABT
NASA Toxicologist

5/1/2019
Date

Concurrence by Valerie Ryder, Ph.D., DABT
NASA Toxicologist

5/1/2019
Date

Enclosures
Table 1A: Analytical concentrations of compounds quantified in the mGSC returned on SpaceX-15
Table 1B: Analytical concentrations of compounds quantified in mGSCs returned on SpaceX-16
Table 2A: T-values corresponding to concentrations for samples returned on SpX-15 in Table 1A, based on 7-day and 180-day SMACs
Table 2B: T-values corresponding to concentrations from the Lab and Service Module in Table 1B, based on 180-day SMACs
Table 2C: T-values corresponding to concentrations from HTV-7 ingress, based on 7-day and 180-day SMACs
Table 3A: Analytical concentrations of compounds quantified in condensate and wastewater returned on Soyuz 54 and SpaceX-15
Table 3B: Analytical concentrations of compounds quantified in PWD hot and product water samples returned on Soyuz 54

TABLE 1A
ANALYTICAL RESULTS OF SPACEX-15 RETURN

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M3)		
	AQ180282 SN2108 Contingency Node 1, OA-9 Hatch Open 7/02/18 @ 11:20 GMT	**AQ180283 SN2013 LAB 7/10/18 @ 11:46 GMT**	**AQ180284 SN2010 Columbus 7/10/18 @ 11:47 GMT**
TARGET COMPOUNDS (TO-15) **			
1,1,1,2-Tetrafluoroethane (Norflurane)	0.062	0.053	0.054
Propane	<0.025	<0.025	TRACE
Carbonyl sulfide (Carbon oxide sulfide)	TRACE	<0.025	<0.025
Methanol *	**1.0**	**0.77**	**0.65**
Acetaldehyde	0.62	0.66	0.72
2-Methyl-1-propene	TRACE	<0.025	<0.025
Ethanol *	**14**	**11**	**11**
Acetone	0.71	0.32	0.36
2-Propanol (Isopropanol)	0.58	0.38	0.47
Isoprene (2-Methyl-1,3-butadiene)	0.049	0.026	0.028
Methyl acetate	TRACE	<0.025	<0.025
Carbon disulfide	0.12	<0.025	<0.025
1-Propanol	0.045	0.039	0.039
Trimethylsilanol	0.30	0.087	0.13
2-Butanone (Methyl ethyl ketone)	0.028	<0.025	<0.025
Ethyl acetate	0.063	0.043	0.040
1-Butanol	0.14	0.058	0.067
3-Methylhexane	0.034	0.029	0.027
o-Xylene	TRACE	TRACE	TRACE
Decamethylcyclopentasiloxane	0.57	0.30	0.26
Octafluoropropane (Perfluoropropane) *	**150**	**140**	**150**
SPECIAL INTEREST COMPOUNDS ***			
Hexamethylcyclotrisiloxane #	0.41	<0.20	<0.20
NON-TARGET COMPOUNDS ***			
Limonene	0.32	<0.050	<0.050
TOTAL ALCOHOLS PLUS ACETONE	**16**	**12**	**13**
TARGET COMPOUNDS (GC) **			
Methane	52	55	55
Carbon dioxide	8200	7000	7100
Hydrogen	4.6	3.3	3.3
Carbon monoxide	0.70	0.64	0.67
TOTAL CONCENTRATION (NON-METHANE HYDROCARBONS)	**169**	**154**	**164**
TOTAL CONCENTRATION - OFP (NON-METHANE HYDROCARBONS)	**19**	**14**	**14**

* GC/FID data results are in bold

** Quantified using a multi-point calibration

*** Quantified using "B" response factor except where noted; concentrations are estimates only.

Response factor generated from an internal study

< : Value is less than the laboratory reporting limit.

TRACE: Amount detected is sufficient for compound identification only. One-half of the reporting limit was used in the Total Concentration summation.

OFP - Octafluoropropane

TABLE 1B
ANALYTICAL RESULTS OF SPACEX-16 RETURN

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M^3)		
	AQ190014 SN2109 LAB 08/21/18 @ 11:19 GMT	**AQ190015 SN2113 SM 08/21/18 @ 11:22 GMT**	**AQ190016 SN2006 HTV-7 Ingress 09/27/18 @ 19:50 GMT**
TARGET COMPOUNDS (TO-15) **			
Carbonyl sulfide (Carbon oxide sulfide)	<0.025	<0.025	0.042
Isobutane	<0.025	<0.025	0.13
Methanol *	**0.58**	**0.45**	0.62
Acetaldehyde	0.32	0.72	0.20
2-Methyl-1-propene	<0.025	<0.025	0.059
Ethanol *	**8.3**	**15**	0.69
Acetone	0.37	0.25	0.48
Propanal (Propionaldehyde)	<0.025	<0.025	0.029
2-Propanol (Isopropanol) *	0.29	0.36	**1.6**
Isoprene (2-Methyl-1,3-butadiene)	0.053	0.038	<0.025
2-Methyl-2-propanol	<0.025	<0.025	TRACE
Carbon disulfide	<0.025	TRACE	0.14
1-Propanol	0.044	TRACE	0.067
Trimethylsilanol	0.12	0.04	2.4
Butanal (Butyraldehyde)	<0.025	<0.025	TRACE
2-Butanone (Methyl ethyl ketone)	<0.025	<0.025	0.068
Ethyl acetate	0.031	0.053	0.035
1-Butanol	0.047	0.056	0.31
Toluene	<0.025	<0.025	0.19
o-Xylene	<0.050	0.052	<0.050
Decamethylcyclopentasiloxane	0.22	0.38	<0.175
Octafluoropropane (Perfluoropropane) *	**114**	**115**	**3.7**
SPECIAL INTEREST COMPOUNDS			
Hexamethylcyclotrisiloxane #	0.22	0.32	2.0
NON-TARGET COMPOUNDS ***			
Fluorotrimethylsilane	<0.050	<0.050	0.12
Cyclohexane	<0.050	<0.050	0.26
TOTAL ALCOHOLS PLUS ACETONE	**9.6**	**16**	**3.8**
TARGET COMPOUNDS (GC) **			
Methane	61	76	4.0
Carbon dioxide	4900	12100	1500
Hydrogen	3.6	3.0	0.31
Carbon monoxide	1.4	0.82	1.3
TOTAL CONCENTRATION (NON-METHANE HYDROCARBONS)	**124**	**133**	**13**
TOTAL CONCENTRATION - OFP (NON-METHANE HYDROCARBONS)	**11**	**18**	**9.5**

* GC/FID data results are in bold
** Quantified using a multi-point calibration
*** Quantified using "B" response factor except where noted; concentrations are estimates only.
# Response factor generated from an internal study
< : Value is less than the laboratory reporting limit.
TRACE: Amount detected is sufficient for compound identification only. One-half of the reporting limit was used in the Total Concentration summation.
OFP - Octafluoropropane

TABLE 2A
T-VALUES FOR SPACEX-15 RETURN

CHEMICAL CONTAMINANT	T-VALUE (180-d SMAC)		
	AQ180282 SN2108 Contingency Node 1, OA-9 Hatch Open 7/02/18 @ 11:20 GMT	**AQ180283 SN2013 LAB 7/10/18 @ 11:46 GMT**	**AQ180284 SN2010 Columbus 7/10/18 @ 11:47 GMT**
TARGET COMPOUNDS (TO-15)			
1,1,1,2-Tetrafluoroethane (Norflurane)	0.00001	0.00001	0.00001
Propane	ND	ND	0.00000
Carbonyl sulfide (Carbon oxide sulfide)	0.00063	ND	ND
Methanol	0.01134	0.00857	0.00719
Acetaldehyde	0.15616	0.16376	0.18080
2-Methyl-1-propene	0.00054	ND	ND
Ethanol	0.00691	0.00539	0.00557
Acetone	0.01359	0.00615	0.00688
2-Propanol (Isopropanol)	0.00390	0.00252	0.00314
Isoprene (2-Methyl-1,3-butadiene)	0.01650	0.00874	0.00919
Methyl acetate	0.00010	ND	ND
Carbon disulfide	0.10645	ND	ND
1-Propanol	0.00061	0.00053	0.00053
Trimethylsilanol	0.07400	0.02173	0.03265
2-Butanone (Methyl ethyl ketone)	0.00094	ND	ND
Ethyl acetate	0.00035	0.00024	0.00022
1-Butanol	0.00347	0.00145	0.00167
3-Methylhexane	0.00279	0.00246	0.00222
o-Xylene	0.00068	0.00068	0.00068
Decamethylcyclopentasiloxane	0.03798	0.02029	0.01746
Octafluoropropane (Perfluoropropane)	0.00182	0.00166	0.00172
SPECIAL INTEREST COMPOUNDS			
Hexamethylcyclotrisiloxane	0.04581	ND	ND
NON-TARGET COMPOUNDS			
Limonene	0.00282	ND	ND
TARGET COMPOUNDS (GC)			
Methane	0.01477	0.01566	0.01578
Hydrogen	0.01344	0.00956	0.00960
Carbon monoxide	0.04111	0.03786	0.03935
TOTAL T-VALUE	**0.55671**	**0.30725**	**0.33466**

ND : Value is less than the laboratory reporting limit.
Note: Number of decimal places in T-Values do not represent significant figures of measurements.

TABLE 2B
T-VALUES FOR SPACEX-16 RETURN

CHEMICAL CONTAMINANT	T-VALUE (180-d SMAC)	
	AQ190014 SN2109 LAB 08/21/18 @ 11:19 GMT	**AQ190015 SN2113 SM 08/21/18 @ 11:22 GMT**
TARGET COMPOUNDS (TO-15)		
Methanol	0.00649	0.00502
Acetaldehyde	0.08037	0.18006
Ethanol	0.00413	0.00768
Acetone	0.00714	0.00479
2-Propanol (Isopropanol)	0.00190	0.00238
Isoprene (2-Methyl-1,3-butadiene)	0.01775	0.01278
Carbon disulfide	ND	0.01136
1-Propanol	0.00059	0.00017
Trimethylsilanol	0.03002	0.00890
Ethyl acetate	0.00017	0.00029
1-Butanol	0.00118	0.00140
o-Xylene	ND	0.00139
Decamethylcyclopentasiloxane	0.01454	0.02548
Octafluoropropane (Perfluoropropane)	0.00134	0.00136
SPECIAL INTEREST COMPOUNDS		
Hexamethylcyclotrisiloxane	0.02496	0.03555
NON-TARGET COMPOUNDS		
All Non-Target Compounds were below their reporting limit.		
TARGET COMPOUNDS (GC)		
Methane	0.01744	0.02177
Hydrogen	0.01070	0.00884
Carbon monoxide	0.08330	0.04801
TOTAL T-VALUE	**0.30203**	**0.37724**

ND : Value is less than the laboratory reporting limit.
Note: Number of decimal places in T-Values do not represent significant figures of measurements.

TABLE 2C
T-VALUES FOR SPACEX-16 RETURN

CHEMICAL CONTAMINANT	T-VALUE (7- & 180-d)	
	7-d SMAC	180-d SMAC
	AQ190016 SN2006 HTV-7 Ingress 09/27/18 @ 19:50 GMT	AQ190016 SN2006 HTV-7 Ingress 09/27/18 @ 19:50 GMT
TARGET COMPOUNDS (TO-15)		
Carbonyl sulfide (Carbon oxide sulfide)	0.00048	0.00211
Isobutane	0.00066	0.00066
Methanol	0.00686	0.00686
Acetaldehyde	0.04991	0.04991
2-Methyl-1-propene	0.00052	0.00258
Ethanol	0.00034	0.00034
Acetone	0.00921	0.00921
Propanal (Propionaldehyde)	0.00240	0.00240
2-Propanol (Isopropanol)	0.01071	0.01071
2-Methyl-2-propanol	0.00008	0.00010
Carbon disulfide	0.12431	0.12431
1-Propanol	0.00090	0.00090
Trimethylsilanol	0.61031	0.61031
Butanal (Butyraldehyde)	0.00083	0.00083
2-Butanone (Methyl ethyl ketone)	0.00228	0.00228
Ethyl acetate	0.00019	0.00019
1-Butanol	0.00386	0.00772
Toluene	0.01266	0.01266
Octafluoropropane (Perfluoropropane)	0.00004	0.00004
SPECIAL INTEREST COMPOUNDS		
Hexamethylcyclotrisiloxane	0.02252	0.22519
NON-TARGET COMPOUNDS		
Fluorotrimethylsilane	0.03288	0.03288
Cyclohexane	0.00122	0.00122
TARGET COMPOUNDS (GC)		
Methane	0.00114	0.00114
Hydrogen	0.00090	0.00090
Carbon monoxide	0.02014	0.07465
TOTAL T-VALUE	**0.91538**	**1.18013**

ND : Value is less than the laboratory reporting limit.
Note: Number of decimal places in T-Values do not represent significant figures of measurements.

Table 3A: Analytical Concentrations of Compounds Quantified in Condensate and Wastewater Samples Returned on Soyuz 54 & SpaceX-15

Increment					56		
Mission					Soyuz 54		SpaceX-15
Sample Location			Potable Water		WPA Wastewater ORU	WPA Condensate Sample Port	ESA Condensate Heat Exchanger (CHX)
Sample Description				Maximum Contaminant Level Source	WPA Wastewater	US Condensate	Columbus Condensate
Sample Date		Test Conducted by	Maximum Contaminant Level (MCL)		7/10/2018	7/10/2018	7/17/2018
Analysis/Sample ID	Units				WQ180675	WQ180676	WQ180520
Physical Characteristics							
Conductivity	µS/cm	U.S.			173	240	350
pH	pH units	U.S.	4.5-8.5	41000	7.74	7.45	5.99
Anions IC							
Bromide	mg/L	U.S.			< 0.1	< 0.1	0.5
Fluoride	mg/L	U.S.			0.4	0.4	0.4
Phosphate (as P)	mg/L	U.S.			0.2	< 0.1	< 0.1
Cations IC							
Ammonium (as N)	mg/L	U.S.	1	SWEG&41000	22.4	31.8	42.3
Minerals ICPMS							
Calcium	mg/L	U.S.	30	41000	0.18	0.28	0.18
Potassium	mg/L	U.S.	340	41000	0.18	0.24	0.05
Sodium	mg/L	U.S.			0.16	0.22	< 0.01
Trace Metals ICPMS							
Aluminum	µg/L	U.S.			< 10	< 20	11
Boron	µg/L	U.S.			16	54	178
Chromium	µg/L	U.S.	230	41000	< 10	< 20	12
Manganese	µg/L	U.S.	300	SWEG&41000	< 10	< 20	4
Molybdenum	µg/L	U.S.			< 10	< 20	6
Nickel	µg/L	U.S.	300	SWEG&41000	54	168	923
Silver	µg/L	U.S.	400	SWEG&41000	< 10	22	< 4
Zinc	µg/L	U.S.	2,000	SWEG&41000	976	3,350	< 4
Silicon ICPMS							
Silicon	µg/L	U.S.			8,540	12,600	29,600
Total Organic Carbon-Sievers & Total Organic Carbon-OI							
Total Inorganic Carbon (TIC)	mg/L	U.S.			18.1	27.1	4.38
Total Organic Carbon (TOC)	mg/L	U.S.		SWEG / 41000	27.7	134	187
Volatile Organics-Targets							
Acetone	µg/L	U.S.	15,000	SWEG	9	see alcohols	see alcohols
Volatile Organics-Special Interest Compounds (Semi-quantitative)							
Acetaldehyde	µg/L	U.S.			not found	24	15,000
Trimethylsilanol	µg/L	U.S.			210	260	430
Volatile Organics-Non-Targets (estimated conc.)							
Fluorotrimethylsilane	µg/L	U.S.			37	75	not found
Methoxytrimethylsilane	µg/L	U.S.			18	not found	not found
Semi-volatile Organics-Targets							
Benzothiazole	µg/L	U.S.			77	98	76
Decamethylcyclopentasiloxane (DMCPS)	µg/L	U.S.			92	262	256
Dodecamethylcyclohexasiloxane	µg/L	U.S.			< 40	127	233
Methyl sulfone	µg/L	U.S.	1,500,000	interim SWEG (06-2017)	208	192	231
N-n-Butylbenzenesulfonamide	µg/L	U.S.			64	78	79
Tris(2-Chloroethyl)phosphate	µg/L	U.S.			97	106	109
Acid Extractables-EPA 625 List GCMS							
4-Methylphenol (p-Cresol)	µg/L	U.S.			< 40	40	42
Benzoic acid	µg/L	U.S.			< 200	2,620	2,310
Phenol	µg/L	U.S.	4,000	SWEG	< 40	513	501
Base and Neutral Extractables-EPA 625 List GCMS							
Benzyl alcohol	µg/L	U.S.			59	21,600	25,100
bis-(2-Ethylhexyl)phthalate	µg/L	U.S.	20,000/6	SWEG/EPA	< 40	58	< 40
Di-n-butylphthalate	µg/L	U.S.	40,000	SWEG	< 40	226	85
Diethylphthalate	µg/L	U.S.			684	951	1,520
Semi-volatile Organics-Special Interest Compounds (Semi-quantitative)							
1,3,5-Triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	µg/L	U.S.			< 40	46	140
1-Methyl-2-pyrrolidinone	µg/L	U.S.			not found	610	960
2-(2-Butoxyethoxy)ethanol	µg/L	U.S.			not found	1,200	1,800
2-Butoxyethanol	µg/L	U.S.			not found	290	220
2-Ethoxyethanol	µg/L	U.S.			not found	500	not found
2-Ethyl-1-hexanol	µg/L	U.S.			not found	360	380
2-Ethylhexanoic acid	µg/L	U.S.			not found	not found	740
2-Methyl-2,4-pentanediol	µg/L	U.S.			110	130	not found

Table 3A: Analytical Concentrations of Compounds Quantified in Condensate and Wastewater Samples Returned on Soyuz 54 & SpaceX-15

Increment					56		
Mission					Soyuz 54		SpaceX-15
Sample Location			Potable Water		WPA Wastewater ORU	WPA Condensate Sample Port	ESA Condensate Heat Exchanger (CHX)
Sample Description				Maximum Contaminant Level Source	WPA Wastewater	US Condensate	Columbus Condensate
Sample Date		Test Conducted by	Maximum Contaminant Level (MCL)		7/10/2018	7/10/2018	7/17/2018
Analysis/Sample ID	Units				WQ180675	WQ180676	WQ180520
2-Phenoxyethanol	µg/L	U.S.			230	1,900	680
2-Phenyl-2-propanol	µg/L	U.S.			160	240	230
Acetophenone	µg/L	U.S.			not found	25	29
Benzaldehyde	µg/L	U.S.			not found	130	200
Butylated hydroxyanisole (BHA)	µg/L	U.S.			210	330	< 80
Heptanoic acid	µg/L	U.S.			not found	not found	450
Hexanoic acid (Caprolate)	µg/L	U.S.			not found	not found	1,100
Methyl 4-hydroxybenzoate	µg/L	U.S.			not found	not found	59
Monomethyl phthalate	µg/L	U.S.			230	390	not found
N,N-Diethylformamide	µg/L	U.S.			not found	not found	89
N,N-Dimethyl acetamide	µg/L	U.S.			540	760	1,400
N,N-Dimethylformamide	µg/L	U.S.			400	660	750
Neomenthol	µg/L	U.S.			61	75	74
Nonanoic acid	µg/L	U.S.			not found	not found	1,400
p-Menth-1-en-8-ol (alpha-Terpineol)	µg/L	U.S.			40	79	not found
Phenethyl alcohol	µg/L	U.S.			not found	52	not found
Tributyl phosphate	µg/L	U.S.			50	63	67
Triethyl phosphate	µg/L	U.S.			not found	not found	53
Alcohols & Acetone GCMS							
1-Butanol	µg/L	U.S.			< 400	476	< 400
1-Propanol	µg/L	U.S.			< 400	608	< 400
2-Propanol (Isopropanol)	µg/L	U.S.			< 400	1,170	4,240
Acetone	µg/L	U.S.	15000	SWEG	see volatiles	3,810	1,110
Ethanol	µg/L	U.S.			< 400	101,000	< 400
Methanol	µg/L	U.S.	40,000	SWEG	3,850	8,540	< 400
Glycols GCMS							
1,2-Ethanediol (Ethylene glycol)	µg/L	U.S.	4000	SWEG	< 1000	2,830	6,770
1,2-Propanediol (Propylene glycol)	µg/L	U.S.	1,700,000	SWEG	< 1000	12,000	15,100
Silanols LCRI (Semi-Quantitative-NIST traceable standard not available)							
Dimethylsilanediol (DMSD)	µg/L	U.S.	35,000	SWEG	25,000	38,000	60,000
Carboxylates IC							
Acetate	µg/L	U.S.			< 500	< 500	161,000
Lactate	µg/L	U.S.			< 500	< 500	903
Aldehydes GCMS							
Formaldehyde	µg/L	U.S.	12,000	SWEG	< 10	32	21
Non-volatile Organics LC							
Caprolactam	µg/L	U.S.	100,000	SWEG	< 500	< 500	2,470
Organic Carbon Recovery	percent	U.S.			36.07	75.76	71.69
Unaccounted Organic Carbon	mg/L	U.S.			17.71	32.48	52.94

Comments: None

Data Qualifiers:
WQ180675: Methyl sulfone - Possible slight low bias; DMSD reanalyzed on 11/6/18 and confirmed by GCMS.
WQ180676: Methyl sulfone - Possible slight low bias
WQ180520: Methanol - Data qualifier: Possible low bias (MS Rec. 74.3%)

Table 3B: Analytical Concentrations of Compounds Quantified in PWD Hot and Product Water Samples Returned on Soyuz 54

Increment					56		
Mission					Soyuz 54		
Sample Location			Potable Water		WPA PWD Hot	Stagnant Leg of Potable BUS in US Lab	Stagnant Leg of Potable Bus in US Lab
Sample Description					Potable water	WPA Product water, Pre-Flush	WPA Product water, Post-Flush
Sample Date					9/10/2018	7/26/2018	7/26/2018
Analysis/Sample ID	Units	Test Conducted by	Maximum Contaminant Level (MCL)	Maximum Contaminant Level Source	WQ180672	WQ180673	WQ180674
Physical Characteristics							
Conductivity	µS/cm	U.S.			2	6	2
pH	pH units	U.S.	4.5-8.5	41000	6.21	5.23	5.23
Iodine LCV							
Iodide	mg/L	U.S.			< 0.05	3.73	0.50
Iodine	mg/L	U.S.			< 0.05	< 0.05	1.34
Total I	mg/L	U.S.	6/0.2	41000 (tl I max/tl I at pt of consumption)	< 0.05	3.78	1.83
Trace Metals ICPMS							
Nickel	µg/L	U.S.	300	SWEG& 41000	4	1,800	46
Silicon ICPMS							
Silicon	µg/L	U.S.			39	71	822
Total Organic Carbon-Sievers & Total Organic Carbon-OI							
Total Inorganic Carbon (TIC)	mg/L	U.S.			0.94	1.22	0.82
Total Organic Carbon (TOC)	mg/L	U.S.		SWEG / 41000	0.42	0.86	1.17
Semi-volatile Organics-Targets							
Methyl sulfone	µg/L	U.S.	1,500,000	**interim SWEG (06-2017)**	150	NA	NA
Base and Neutral Extractables-EPA 625 List GCMS							
Benzyl alcohol	µg/L	U.S.			24	NA	NA
Silanols LCRI (Semi-Quantitative-NIST traceable standard not available)							
Dimethylsilanediol (DMSD)	µg/L	U.S.	35,000	SWEG	< 1000	< 1000	2,700
Organic Carbon Recovery	percent	U.S.			13.6	N/A	N/A
Unaccounted Organic Carbon	mg/L	U.S.			0.36	N/A	N/A

Comments: NA=Not analyzed; N/A=Not applicable

Data Qualifiers: WQ180672: Methyl sulfone - Possible slight low bias