JSC TOXICOLOGY GROUP

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SUBJECT: Toxicological Assessment of SpaceX-5 (SpX-5) First Ingress Air Quality and Node 3 Contingency Air Sample

SUMMARY: *SpX-5 first ingress* - The T-value measured at first entry met acceptable limits and does not pose a concern for crew health.
Node 3 contingency - One of the non-target compounds (isoprene) may have contributed to the odors that prompted the contingency sampling, but none of the compounds measured were at levels of concern for crew health.

One mini-grab sample container (m-GSC) was collected by crew members onboard ISS during first ingress into SpX-5 on January 13, 2015. The ingress sample was collected approximately 8 minutes after hatch opening and approximately 84 hours after the pre-launch clean air purge. An additional m-GSC was collected on January 18, 2015 after crew reports of a burning odor in Node 3. Both samples were returned on SpX-5.

Routine monthly sampling in the US Lab and alternating between the Russian Service Module, European Columbus module, and the Japanese Pressurized Module was originally scheduled for January 5, 2015. This sampling session was postponed until after the arrival of SpX-5 to enable concurrent formaldehyde sampling, but the cargo transfer schedule resulted in a substantial delay and cancellation of the January sampling session.

A summary of the analytical results for the samples returned on SpX-5 is shown in Table 1. Complete data tables of all measured concentrations are enclosed. A corresponding table of T-values calculated using both the 7-day and 180-day SMACs for the first ingress sample are also enclosed. No T-value table is provided for the contingency sample because short-term SMACs are not available for all compounds detected. The average relative recoveries of the 3 surrogate standards from the mGSCs were as follows: ^{13}C-acetone, 109 ± 7%; fluorobenzene-d5, 109 ± 9%; and chlorobenzene-d5, 101 ± 17%. Initial sample pressures were 14.4 and 14.3 psia for the ingress and contingency samples, respectively, indicating nominal sample collection.

Table 1. Analytical Summary of ISS results

Sample Location	Sample Date	NMVOCs[a] (mg/m^3)	Freon 218 (mg/m^3)	CO_2 (mg/m^3)	Alcohols[b] (mg/m^3)	T-value[c] (units)
SpaceX-5 first ingress	1/13/2015	131	136	4900	10	0.5 (1.2)
Node 3 contingency	1/18/2015	15	268	7700	11	--
Guideline		*<25*	---	*<9300*	*<5*	*<3*

[a]Non-methane volatile organic hydrocarbons, excluding Freon 218
[b]Includes acetone
[c]Based on 7-d SMACs and calculated excluding CO_2; parentheses indicate value based on 180-day SMACs

Toxicological Evaluation of ISS Air Quality

SpX-5 First Ingress

Although the sample was collected within ~8 minutes of hatch opening, the volume of the commercial vehicles is quite small (~10m^3), and reported CO_2 and Freon 218 levels indicate substantial mixing with the ISS atmosphere. As a result, the data may underrepresent contaminant levels at docking. Despite this, the total contaminant load (NMVOC) was much higher than that seen for recent SpaceX vehicles. The elevated levels are primarily due to perfluoro-2-methylpentane, which originates from the heat-exchange fluid used by the Dragon vehicle. This compound was below the limit of detection for SpX-4, but was measured at 110 mg/m^3 in this sample. This concentration is higher than any SpaceX vehicle since the demonstration mission where the coolant leak was first identified. Substantially reduced, but measurable levels (0.7 mg/m^3) of this compound were detected in the Node 3 contingency sample collected 5 days later, which is consistent with dilution across the ISS stack. This information has been conveyed to ON who has agreed to coordinate with SpaceX to ensure that the leak is mitigated prior to the launch of SpX-7. The primary contributors to the T-value were trimethylsilanol (TMS), hexamethylcyclotrisiloxane (HMCTS), and acetaldehyde. The TMS concentration remained below levels of concern for crew health but was 10-fold higher than the concentration measured on SpX-4. In addition, there were a number of non-target compounds detected that were not seen in previous SpaceX first ingress samples, including dodecafluoropentane, 1,1,1,2-tetrafluoroethane (R-134a), cyclohexane, and several medium chain alkanes. Concentrations of these compounds were very low, but potential sources, especially of the R-134a refrigerant, will be investigated.

Node 3 Contingency Sample

Concentrations of target compounds in the Node 3 contingency sample did not differ substantially from background ISS levels with the exception of dichloromethane and o-xylene, which were only slightly elevated, and Freon 218, which was notably elevated. The likely source of the Freon 218 is an estimated leak of 100 g of the coolant from the CKB on 11/19/2014. The only non-target compounds detected were isoprene and R-134a. The refrigerant was present in the SpX-5 ingress sample, and therefore was not likely attributable to the contingency event. Isoprene, a component of synthetic rubber, was reported just above the detection limit of 0.05 mg/m^3. The odor threshold for isoprene is 0.005 ppm or 0.01 mg/m^3, so it is possible that isoprene contributed to the odor the crew noted. However, the concentration remains below the 180-day SMAC value of 3 mg/m^3 and well below the contingency (1-hr) SMAC value of 140 mg/m^3 and is not a concern for crew health.

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5/15/15

Date

Enclosures Table 1: Analytical concentrations of compounds found in the first ingress and contingency m-GSCs
Table 2: T-values corresponding to analytical concentrations in Table 1, based on 7-day and 180-day SMACs for the first ingress GSC

TABLE 1
ANALYTICAL RESULTS OF
SPACEX-5 RETURN GSC AIR SAMPLES

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M^3)	
	AA05877 SN 2078 SpaceX-5 Ingress 1/13/15 @ 08:30 GMT	AA05878 SN 2079 Node 3 Contingency 1/18/15 @ 12:20 GMT
TARGET COMPOUNDS (TO-15)		
FREON12	<0.025	<0.025
CHLOROMETHANE	TRACE	<0.025
FREON114	<0.025	<0.025
METHANOL	0.43	0.24
ACETALDEHYDE	0.24	0.29
VINYLCHLORIDE	<0.025	<0.025
BROMOMETHANE	<0.025	<0.025
ETHANOL *	**5.4**	**10**
CHLOROETHANE	<0.025	<0.025
ACETONITRILE	<0.025	<0.025
PROPENAL	<0.025	<0.025
ACETONE	0.42	0.36
PROPANAL	0.026	<0.025
ISOPROPANOL *	**2.9**	0.27
FREON11	<0.025	<0.025
FURAN	<0.025	<0.025
ACRYLONITRILE	<0.025	<0.025
PENTANE	<0.025	<0.025
2-METHYL-2-PROPANOL	0.038	<0.025
METHYLACETATE	<0.025	TRACE
1,1-DICHLOROETHENE	<0.025	<0.025
DICHLOROMETHANE	0.026	0.037
3-CHLOROPROPENE	<0.025	<0.025
FREON113	<0.025	<0.025
N-PROPANOL	0.050	0.025
1,1-DICHLOROETHANE	<0.025	<0.025
BUTANAL	TRACE	<0.025
2-BUTANONE	0.14	TRACE
CIS-1,2-DICHLOROETHENE	<0.025	<0.025
2-METHYLFURAN	<0.025	<0.025
ETHYLACETATE	0.15	0.040
HEXANE	<0.025	<0.025
CHLOROFORM	<0.025	<0.025
2-BUTENAL	<0.025	<0.025
1,2-DICHLOROETHANE	<0.025	TRACE
1,1,1-TRICHLOROETHANE	<0.025	<0.025
N-BUTANOL	0.72	0.060
BENZENE	<0.025	<0.025
CARBONTETRACHLORIDE	<0.025	<0.025
2-PENTANONE	<0.025	<0.025
2-METHYLHEXANE	TRACE	<0.025
2,3-DIMETHYLPENTANE	<0.025	<0.025
PENTANAL	<0.025	<0.025
3-METHYLHEXANE	TRACE	<0.025
1,2-DICHLOROPROPANE	<0.025	<0.025
1,4-DIOXANE	<0.025	<0.025
TRICHLOROETHENE	<0.025	<0.025
2,5-DIMETHYLFURAN	<0.025	<0.025
N-HEPTANE	<0.025	<0.025
4-METHYL2-PENTANONE	0.046	<0.025
CIS-1,3-DICHLOROPROPENE	<0.025	<0.025
2-PENTENAL	<0.025	<0.025
TRANS-1,3-DICHLOROPROPENE	<0.025	<0.025
1,1,2-TRICHLOROETHANE	<0.025	<0.025
TOLUENE	0.19	TRACE
HEXANAL	TRACE	<0.025
MESITYLOXIDE	<0.025	<0.025
1,2-DIBROMOETHANE	<0.025	<0.025
BUTYLACETATE	0.074	<0.025
OCTANE	<0.025	<0.025
TETRACHLOROETHENE	<0.025	<0.025
CHLOROBENZENE	<0.025	<0.025
ETHYLBENZENE	0.11	<0.025
M/P-XYLENES	0.11	<0.050
2-HEPTANONE	<0.025	<0.025
CYCLOHEXANONE	<0.025	<0.025
HEPTANAL	<0.025	<0.025
STYRENE	<0.025	<0.025
1,1,2,2-TETRACHLOROETHANE	<0.025	<0.025
O-XYLENE	0.080	0.027
NONANE	<0.025	<0.025
1,3,5-TRIMETHYLBENZENE	<0.025	<0.025
1,2,4-TRIMETHYLBENZENE	<0.025	<0.025
1,3-DICHLOROBENZENE	<0.025	<0.025
1,4-DICHLOROBENZENE	<0.025	<0.025
1,2-DICHLOROBENZENE	<0.025	<0.025
1,2,4-TRICHLOROBENZENE	<0.050	<0.050
HEXACHLORO-1,3-BUTADIENE	<0.075	<0.075

TABLE I
ANALYTICAL RESULTS OF
SPACEX-5 RETURN GSC AIR SAMPLES

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M^3)	
	AA05877 SN 2078 SpaceX-5 Ingress 1/13/15 @ 08:30 GMT	AA05878 SN 2079 Node 3 Contingency 1/18/15 @ 12:20 GMT
SPECIAL INTEREST COMPOUNDS **		
1,3-BUTADIENE &	<0.050	<0.050
ETHYLENE OXIDE	<0.050	<0.050
2-METHYL-2-PROPENAL	<0.050	<0.050
3-BUTEN-2-ONE	<0.050	<0.050
2-ETHOXYETHANOL	<0.050	<0.050
DIMETHYL DISULFIDE	<0.050	<0.050
OCTAFLUOROPROPANE & *	**136**	**268**
PERFLUORO-2-METHYLPENTANE & *	**110**	0.72
CARBONYL SULFIDE &	0.026	<0.025
ISOBUTANE &	0.4	<0.025
2-METHYL-1-PROPENE &	0.044	TRACE
DIMETHYL SULFIDE &	<0.025	<0.025
CARBON DISULFIDE &	TRACE	<0.025
TRIMETHYLSILANOL &	0.71	0.069
OCTAMETHYLCYCLOTETRASILOXANE &	0.09	<0.075
DECAMETHYLCYCLOPENTASILOXANE &	0.18	0.28
HEXAMETHYLCYCLOTRISILOXANE %	6.3	2.0
NON-TARGET COMPOUNDS **		
PROPENE &	<0.050	<0.050
PROPANE &	TRACE	<0.050
BUTANE &	<0.050	<0.050
ISOPRENE &	TRACE	0.051
DODECAFLUOROPENTANE	0.32	<0.050
1,1,1,2-TETRAFLUOROETHANE	0.32	0.10
UNIDENTIFIED FLUORINATED COMPOUND	<0.050	<0.050
CYCLOHEXANE	0.068	<0.050
METHYLCYCLOHEPTANE	<0.050	<0.050
C3-SUBSTITUTED CYCLOPENTANE	<0.050	<0.050
C9-ALKANE	<0.050	<0.050
C3-SUBSTITUTED CYCLOHEXANE	TRACE	<0.050
C11-ALKANE	0.078	<0.050
C12-ALKANE	0.051	<0.050
C12-ALKANE	0.15	<0.050
2-ETHYL-1-HEXANOL	TRACE	<0.050
C12-ALKANE	0.068	<0.050
C4-SUBSTITUTED BENZENE	<0.050	<0.050
C12-ALKANE	0.20	<0.050
LIMONENE	0.13	TRACE
C12-ALKANE	<0.050	<0.050
C12-ALKANE	0.15	<0.050
C12-ALKANE	0.16	<0.050
C12-ALKANE	0.052	<0.050
C12-ALKANE	<0.050	<0.050
TOTAL ALCOHOLS PLUS ACETONE	**10**	**11**
TARGET COMPOUNDS (GC)		
CARBON MONOXIDE	1.0	0.36
METHANE	2.6	2.9
HYDROGEN	4.4	6.4
CARBON DIOXIDE	4863	7659
TOTAL CONCENTRATION (NON-METHANE HYDROCARBONS)	**267**	**283**
TOTAL CONCENTRATION - OFP (NON-METHANE HYDROCARBONS)	**131**	**15**

* GC/FID data results are in bold

** Quantified using "B" response factor except where noted

& Quantified using a multi-point calibration

% Response factor generated from an internal study

< : Value is less than the laboratory report detection limit.

TRACE: Amount detected is sufficient for compound identification only.

OFP - Octafluoropropane

TABLE 2
T-VALUES FOR
SPACEX-5 INGRESS GSC AIR SAMPLES

CHEMICAL CONTAMINANT	AA05877 SN 2078 SpaceX-5 Ingress 1/13/15 @ 08:30 GMT	
	T-VALUE (7-d SMAC)	T-VALUE (180-d SMAC)
TARGET COMPOUNDS (TO-15)		
FREON12	ND	ND
CHLOROMETHANE	0.00030	0.00030
FREON114	ND	ND
METHANOL	0.00480	0.00480
ACETALDEHYDE	0.05932	0.05932
VINYLCHLORIDE	ND	ND
BROMOMETHANE	ND	ND
ETHANOL	0.00270	0.00270
CHLOROETHANE	ND	ND
ACETONITRILE	ND	ND
PROPENAL	ND	ND
ACETONE	0.00813	0.00813
PROPANAL	0.00239	0.00239
ISOPROPANOL	0.01948	0.01948
FREON11	ND	ND
FURAN	ND	ND
ACRYLONITRILE	ND	ND
PENTANE	ND	ND
2-METHYL-2-PROPANOL	0.00025	0.00032
METHYLACETATE	ND	ND
1,1-DICHLOROETHENE	ND	ND
DICHLOROMETHANE	0.00054	0.00263
3-CHLOROPROPENE	ND	ND
FREON113	ND	ND
N-PROPANOL	0.00051	0.00051
1,1-DICHLOROETHANE	ND	ND
BUTANAL	0.00096	0.00096
2-BUTANONE	0.00465	0.00465
CIS-1,2-DICHLOROETHENE	ND	ND
2-METHYLFURAN	ND	ND
ETHYLACETATE	0.00082	0.00082
HEXANE	ND	ND
CHLOROFORM	ND	ND
2-BUTENAL	ND	ND
1,2-DICHLOROETHANE	ND	ND
1,1,1-TRICHLOROETHANE	ND	ND
N-BUTANOL	0.00897	0.01795
BENZENE	ND	ND
CARBONTETRACHLORIDE	ND	ND
2-PENTANONE	ND	ND
2-METHYLHEXANE	0.00005	0.00104
2,3-DIMETHYLPENTANE	ND	ND
PENTANAL	ND	ND
3-METHYLHEXANE	0.00005	0.00104
1,2-DICHLOROPROPANE	ND	ND
1,4-DIOXANE	ND	ND
TRICHLOROETHENE	ND	ND
2,5-DIMETHYLFURAN	ND	ND
N-HEPTANE	ND	ND
4-METHYL2-PENTANONE	0.00033	0.00033
CIS-1,3-DICHLOROPROPENE	ND	ND
2-PENTENAL	ND	ND
TRANS-1,3-DICHLOROPROPENE	ND	ND
1,1,2-TRICHLOROETHANE	ND	ND
TOLUENE	0.01297	0.01297
HEXANAL	0.00069	0.00069
MESITYLOXIDE	ND	ND
1,2-DIBROMOETHANE	ND	ND
BUTYLACETATE	0.00039	0.00039
OCTANE	ND	ND
TETRACHLOROETHENE	ND	ND
CHLOROBENZENE	ND	ND
ETHYLBENZENE	0.00085	0.00222
M/P-XYLENES	0.00157	0.00311
2-HEPTANONE	ND	ND
CYCLOHEXANONE	ND	ND
HEPTANAL	ND	ND
STYRENE	ND	ND
1,1,2,2-TETRACHLOROETHANE	ND	ND
O-XYLENE	0.00109	0.00215
NONANE	ND	ND
1,3,5-TRIMETHYLBENZENE	ND	ND
1,2,4-TRIMETHYLBENZENE	ND	ND
1,3-DICHLOROBENZENE	ND	ND
1,4-DICHLOROBENZENE	ND	ND
1,2-DICHLOROBENZENE	ND	ND
1,2,4-TRICHLOROBENZENE	ND	ND
HEXACHLORO-1,3-BUTADIENE	ND	ND

TABLE 2
T-VALUES FOR
SPACEX-5 INGRESS GSC AIR SAMPLES

CHEMICAL CONTAMINANT	AA05877 SN 2078 SpaceX-5 Ingress 1/13/15 @ 08:30 GMT	
	T-VALUE (7-d SMAC)	T-VALUE (180-d SMAC)
SPECIAL INTEREST COMPOUNDS		
1,3-BUTADIENE	ND	ND
ETHYLENE OXIDE	ND	ND
2-METHYL-2-PROPENAL	ND	ND
3-BUTEN-2-ONE	ND	ND
2-ETHOXYETHANOL	ND	ND
DIMETHYL DISULFIDE	ND	ND
OCTAFLUOROPROPANE	0.00160	0.00160
PERFLUORO-2-METHYLPENTANE	0.00735	0.00074
CARBONYL SULFIDE	0.00219	0.00219
ISOBUTANE	0.00166	0.00166
2-METHYL-1-PROPENE	0.00004	0.00004
DIMETHYL SULFIDE	ND	ND
CARBON DISULFIDE	0.00078	0.00078
TRIMETHYLSILANOL	0.17763	0.17763
OCTAMETHYLCYCLOTETRASILOXANE	0.00031	0.00714
DECAMETHYLCYCLOPENTASILOXANE	0.00176	0.01175
HEXAMETHYLCYCLOTRISILOXANE	0.07020	0.70201
NON-TARGET COMPOUNDS		
PROPENE	ND	ND
PROPANE	0.00023	0.00455
BUTANE	ND	ND
ISOPRENE	0.00417	0.00833
DODECAFLUOROPENTANE	0.00109	0.00109
1,1,1,2-TETRAFLUOROETHANE	0.00303	0.00303
UNIDENTIFIED FLUORINATED COMPOUND	ND	ND
CYCLOHEXANE	0.00032	0.00032
METHYLCYCLOHEPTANE	ND	ND
C3-SUBSTITUTED CYCLOPENTANE	ND	ND
C9-ALKANE	ND	ND
C3-SUBSTITUTED CYCLOHEXANE	0.00064	0.00064
C11-ALKANE	0.00162	0.00162
C12-ALKANE	0.00098	0.00098
C12-ALKANE	0.00287	0.00287
2-ETHYL-1-HEXANOL	0.00047	0.00047
C12-ALKANE	0.00131	0.00131
C4-SUBSTITUTED BENZENE	ND	ND
C12-ALKANE	0.00385	0.00385
LIMONENE	0.00110	0.00110
C12-ALKANE	ND	ND
C12-ALKANE	0.00293	0.00293
C12-ALKANE	0.00312	0.00312
C12-ALKANE	0.00100	0.00100
C12-ALKANE	ND	ND
TARGET COMPOUNDS (GC)		
CARBON MONOXIDE	0.01663	0.06163
METHANE	0.00075	0.00075
HYDROGEN	0.01305	0.01305
CARBON DIOXIDE	0.37411	0.37411
TOTAL T-VALUE	**0.82863**	**1.54120**
TOTAL T-VALUE - CO2	**0.45452**	**1.16708**

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