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Quantitative Measurements of Hazardous Gas Effluents from the Combustion of Crew Waste Simulant in Microgravity

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Abstract

In August 2021, Blue Origin launched their un-crewed NS-17 mission aboard their New Shepard launch vehicle. Among the scientific payloads was NASA's Orbital Syngas Commodity Augmentation Reactor (OSCAR), a flight-capable test rig allowing the combustion of ~10 g of simulated astronaut trash. Developed at NASA's Kennedy Space Center, OSCAR measured differences in the combustion of complex mixed waste materials between terrestrial gravity and microgravity conditions. OSCAR is self-contained and collects its own effluent gases, which were subsequently analyzed for trace volatile organic compounds (VOCs) with a modified EPA Method TO-15. It was found that combustion in microgravity produced higher levels of VOCs (2,883 mg measured VOCs per kg trash) than for analogous triplicate (terrestrial) laboratory experiments (1,237±286 mg measured VOCs per kg trash with 95% confidence interval), indicating significant differences that were consistent with previously reported combustion efficiencies. Also, the concentrations of the measured VOCs were compared to NASA's Spacecraft Maximum Allowable Concentrations (SMAC) values. These results provide a basis for understanding important design considerations for spacecraft waste disposal systems as NASA and their commercial partners develop crewed vehicles for missions to the Moon and Mars.

Keywords

volatile organic compounds • combustion • microgravity • trace gas analysis • spacecraft maximum allowable concentrations (SMAC) • TO-15.

Introduction

Current planning for crewed space exploration is being developed within the 'Moon-to-Mars' framework (NASA, 2023). Although the most immediate and visible activity within this framework is exemplified by the Artemis missions, planning for crewed missions to Mars is underway. Proposed Mars mission durations range from 700 to 1,200 days; thus, intensive consideration of mission logistics is required for such a mission to be feasible (Chai et al., 2021). NASA's Logistics Reduction program is currently evaluating numerous facets of mission logistics, including supply organization via RFID technology (Fink et al., 2017), crew clothing and laundry (Ewert and Jeng 2015; Broyan, Chu, and Ewert 2014), handling of metabolic waste (McKinley, Borrego, and Broyan, 2022), re-purposing waste items (Shull, Polit Casillas, and Howe 2012), and disposal of crew trash (Anthony and Hintze 2014; J. Olson et al. 2021; Wetzel et al. 2018; Mesa et al. 2021; Sepka et al. 2022). Among these, the authors have performed several studies on the disposal of crew trash via the so-called Trash-to-Gas (TtG) approach (Pitts et al. 2022; Meier et al. 2021; 2020; Shah, Meier, and Toro Medina 2019). In this paradigm, a thermal process is used to convert solid crew trash into a relatively inert gas that can be safely vented into space, thus reducing the total mass of a vehicle and, correspondingly, reducing the propellant required for mission maneuvers (e.g., orbit insertions and transit injections) (J. A. Olson et al. 2021). Various thermal processes have been investigated by NASA and via public-private SBIR partnerships, including combustion/incineration, steam reforming, pyrolysis, torrefaction, and plasma processes (combustion and pyrolysis) (J. Olson et al., 2021). It is projected that the thermal processing of crew trash could result in substantial mass savings of >6,000 kg for a Mars transit vehicle, representing more than 13% of the payload mass (J. A. Olson et al., 2021). Such mass savings are highly desirable since they would allow for additional valuable (e.g., scientific) payloads. TtG systems may also be applicable to a sustained lunar presence, which is expected beyond the three currently planned Artemis missions (U.S. Government, 2020). A critical consideration for a TtG system is the possibility of contaminating the habitable volume with volatile organic compounds (VOCs). The purpose of this study is to compare the

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combustion VOCs produced under microgravity vs. analogous terrestrial laboratory tests to evaluate potential differences in performance.

Researchers at NASA's Kennedy Space Center (Florida, USA) have undertaken several TtG test campaigns wherein the combustion of simulated crew trash was performed under microgravity conditions to determine the feasibility of such an operation and to compare trash combustion in a terrestrial venue versus microgravity (Pitts et al. 2022; Meier et al. 2021; 2020; Shah, Meier, and Toro Medina 2019). The system for these studies is the Orbital Syngas Commodity Augmentation Reactor (OSCAR) (Toro Medina et al. 2020). As described below, OSCAR is a flight-capable subscale TtG system designed to perform tests in microgravity as well as under terrestrial laboratory conditions to provide a direct experimental comparison of performance. OSCAR utilized combustion during the microgravity demonstration described here due to time constraints inherent in sub-orbital flight, but it can perform various thermal degradation processes. The OSCAR microgravity test activities have included two drop-tower campaigns (at Glenn Research Center, Cleveland, OH, USA) and two flights on board Blue Origin's New Shepard spacecraft (from Blue Origin's Launch Site One, in Van Horn, TX, USA) (Meier et al. 2020; Shah, Meier, and Toro Medina 2019; Meier et al. 2021). While the drop-tower campaigns provided microgravity durations of seconds, the New Shepard vehicle provided over three minutes of microgravity, wherein a substantial amount of simulated waste material (~10 g) was combusted. The results presented here are from the second flight test, after which gas samples were collected for trace gas analyses using a single combustion test. Also note that, due to test differences and anomalies (especially in the first OSCAR flight test), it is difficult to draw direct comparisons between the two flight tests.

NASA has pursued analyses of combustion in space on board the International Space Station (ISS) and associated vehicles. While the primary motivation for these studies is the evaluation of spacecraft fire hazards, they are also of interest for their contribution toward understanding fundamental aspects of the behavior of flames. Combustion testing on board the ISS is complicated by the significant crew hazard associated with it. Thus, much previous work was with small amounts of fuel, and under very strictly controlled self-contained atmospheres (Irace et al. 2021; Sandra L. Olson and Ferkul 2017; D. L. Dietrich et al. 2017; Ma et al. 2015; Daniel L. Dietrich et al. 2014; D.L. Dietrich et al. 2000; Nayagam et al. 1998). More recently, as part of NASA's Saffire Project, larger amounts of fuel (56 g of cotton) were combusted in microgravity in the uncrewed Cygnus logistics module after separation from the ISS (Sandra L. Olson et al. 2023; Thomsen et al. 2022; Li and Liao 2021). These studies revealed important differences between combustion under conditions of terrestrial gravity versus microgravity. Under microgravity conditions, a flame cannot generate the convective flow resulting from the natural buoyancy of the heated effluent gases; thus, quiescent microgravity combustion results in a diffusion-limited condition. To compensate, several microgravity studies (such as Saffire) utilized forced flow to compare with terrestrial buoyant convection (Sandra L. Olson and Ferkul 2017; Thomsen et al. 2022; Li and Liao 2021; Urban et al. 2019). While these studies have provided excellent insight into combustion under microgravity and have informed the designs of more practical combustion devices, note that they used controlled experimental arrangements utilizing 1- or 2-dimensional single-component fuels with (typically) imposed flow parallel to the fuel surfaces. Though very informative, it is not clear whether these results are applicable to the combustion of mixed materials, such as a comprehensive crew waste stream. Additionally, while forced flow can be designed into a trash reactor, it will not have controlled gas flow over all fuel surfaces. The combustion of trash in microgravity represents a more complex process and provides the motivation for the OSCAR test campaigns.

For crew safety, NASA pays careful attention to the constituents in spacecraft cabin air and maintains a list of potentially hazardous and ubiquitous compounds of greatest concern called the Spacecraft Maximum Allowable Concentrations for Airborne Contaminants (SMAC) list (Ryder 2022). The SMAC list includes exposure limits that have been determined from careful appraisal of the physiological effects of the contaminants. The SMAC list includes 56 entries (see Supporting Information) encompassing 70 individual chemical species, including 64 VOCs. Exposure limits are organized according to durations from 1 hour to 1000 days. SMAC exposure limits are not equivalent to other similar measures, such as OSHA's Permissible Exposure Limit (PEL). In general, the SMAC limits decrease (or in some cases remain the same) with increased exposure duration, though some species are not given exposure limits for all durations.

The SMAC list is not exhaustive regarding potential gaseous hazards on a spacecraft. Indeed, analyses of cabin air on the ISS have observed additional contaminants, including 1-propanol, ethyl acetate, R134a, Freon 218, tetramethylsilane, acrylonitrile, and isobutane (Lewis 2015). However, the SMAC list forms the basis for airborne crew hazards and is emphasized here. The analyses described here included other non-SMAC contaminants that are routinely measured on the ISS.

Materials and Methods

As mentioned, the OSCAR system was developed for both flight and laboratory operations; it flew as a payload aboard the

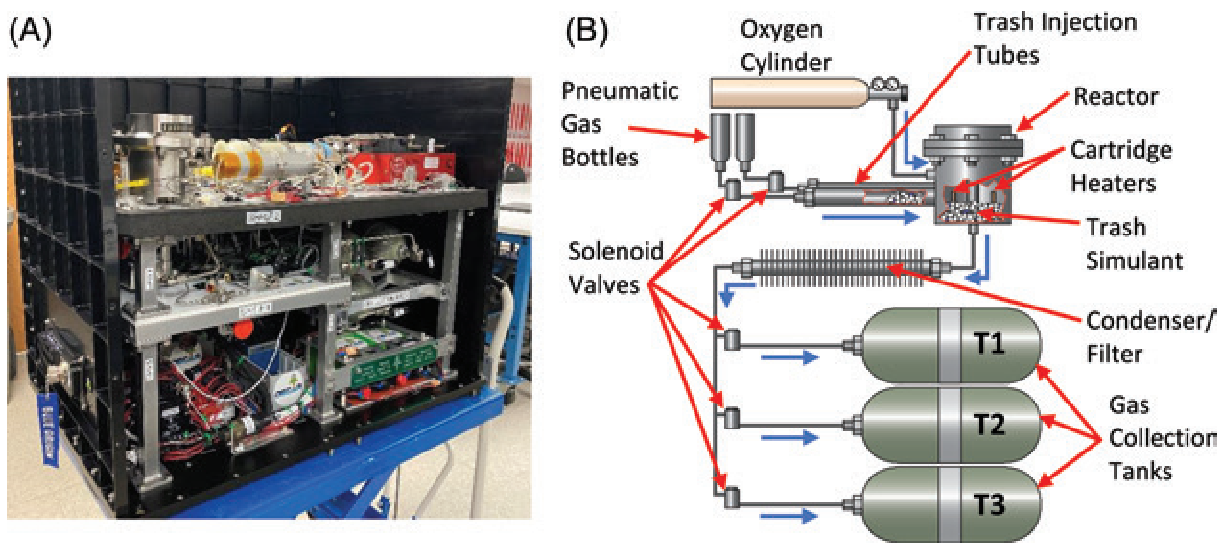

Figure 1. (A) A photograph of the OSCAR system mounted in the flight enclosure prepared for mission NS-17 at the Blue Origin Launch Site One near Van Allen, TX. **(B)** Schematic of the pertinent systems of OSCAR. The blue arrows indicate the direction of gas flow. Note that the gases in the collection tanks were filtered, whereas the gases from the reactor were not.

Blue Origin New Shepard vehicle during the NS-17 mission on August 26, 2021. The flight provided >3 min of microgravity during which it combusted ~10 g of simulated crew trash (Pitts et al. 2022). While pertinent aspects of the OSCAR experiments are described here, the reader is directed to the cited work for a more detailed description of the flight experiment. The OSCAR system is shown in Figure 1(A). Figure 1(B) shows a schematic of the pertinent systems of OSCAR, including the reactor, oxygen supply, trash injection tubes, condenser/filter, and gas collection tanks. For the NS-17 flight, ~8 g of trash simulant was placed into the reactor, and ~1 g of trash simulant was placed into each of two injection tubes, for a total of 10 g (see Supporting Information for a complete description of the waste simulant). Upon achieving microgravity conditions, the reactor was heated, thus initiating the combustion of the trash. The trash from the injection tubes was pneumatically injected into the reactor at set times to sustain the combustion under microgravity. Toward the end of the microgravity phase, solenoid valves opened sequentially to collect the product gases (after filtering via the heat condenser/filter) into collection tanks. Thus, the combustion product gas collection was performed only under microgravity.

The OSCAR reactor/gas system is sealed from the external atmosphere. Feedstock O_2 from a 103 L tank at 1000 psig (6205 kPa) regulated down to 100 psig (589 kPa) supplied oxygen at a constant flow rate of ~3 SLPM owing to a 0.0094" orifice located upstream of the reactor (890 cm^3), and a back pressure regulator set at 30 psig located downstream of the reactor. This higher pressure of pure oxygen was required to complete combustion in the time allowed during the microgravity phase of flight. The rate of flow and reactor volume resulted in a residence time of 139 s. Pure O_2 was used to prime the reactor before ignition and maintain the reaction until all the fuel was consumed. Oxygen entered the reactor from heated feedlines at 650°C at two inlets that were angled tangentially to the reactor circumference to create a gas vortex flow to maximize mixing and compensate for the lack of buoyant convection in microgravity. The reactor reached a maximum temperature of ~800°C.

The combustion gas effluent was passed through a multi-stage heat exchanger/condenser/filter upon exiting the reactor. The first filter was located inside the reactor and consisted of a small metallic 100-mesh screen that prevented unburnt fuel particles from exiting, especially during micro-gravity. The second filter was provided by glass wool at the entrance and exit of the condenser/filter. The condenser/filter was used to filter, condense, and dry the combustion products. Condensation was achieved by passive convection heat transfer via the finned dissipative condenser. Moisture was collected via a 3:1 mass ratio of silica gel and 4A mol sieve 4-8 mesh beads between the glass wool plugs. Lastly, the cooled gas was filtered through a 40 micron-rated sintered stainless-steel filter prior to the collection tanks.

The product gases were sequentially discharged into the three collection tanks (T1-3). T1 was collected before the initiation of combustion and represents a control sample. T2 was collected after combustion was initiated and included the first trash injection tube. T3 was collected after T2 and included the second trash injection tube. Upon flight completion, each collection tank and the reactor remained sealed via the closed solenoid valves.

Table 1. Compounds not observed above the reporting limit, all samples.

Fluorides/Bromides not observed	Polychlorides not observed	
1,1,1,2-tetrafluoroethane	1,1-dichloroethene	*cis*-1,3-dichloropropene
perfluoro-2-methylpentane	Dichloromethane	*trans*-1,3-dichloropropene
dichlorodifluoromethane (Freon 12)	1,1-dichloroethane	1,1,2-trichloroethane
1,2-dichloro-1,1,2,2-tetrafluoroethane (Freon 114)	*cis*-1,2-dichloroethene	tetrachloroethene
trichlorofluoromethane (Freon 11)	chloroform	1,3-dichlorobenzene
1,1,2-trichloro-1,2,2-trifluoroethane (Freon 113)	1,1,1-trichloroethane	1,4-dichlorobenzene
Bromomethane	carbon tetrachloride	1,2-dichlorobenzene
1,2-dibromoethane	trichloroethene	1,2,4-trichlorobenzene
	1,2-dichloropropane	Hexachlorobutadiene

Within ~2 hours post-flight, hand valves were closed to isolate the reactor and the collection tanks that were then retrieved. Samples were then transferred from each collection tank into grab sample containers (GSCs, for trace gas analyses) by connecting directly to each collection tank. A control sample of room air was also collected. The following day, the reactor was retrieved from the New Shepard capsule, whereupon an additional GSC was used to collect gases directly from the reactor. The OSCAR gas system remained under positive pressure after the flight, thus eliminating the possibility of contamination from the atmosphere.

Triplicate analogous terrestrial laboratory tests were completed following the flight operations. These tests were performed with identical timings as for the flight experiment (i.e., actuation of pertinent solenoid valves, duration of heater cartridge actuation, timing of trash injections, etc.). For the lab tests, corresponding gas samples were collected for trace gas analyses. The only procedural difference between laboratory and flight tests was that reactor gases were collected on the same day for the laboratory experiments versus the next day for the flight experiment. However, temperature data indicated that the reactor temperatures were below 100°C for the flight experiment during the time for which laboratory gas samples were collected. Thus, no additional combustion occurred before the collection of the reactor flight gas samples. Gas samples were analyzed by the Environmental Chemistry Laboratory at NASA's Johnson Space Center, Houston, TX.

The preparation of the GSCs included leak checking, cleaning, proofing (verifying cleanliness), evacuating, and dosing with a surrogate. The GSCs were leak-checked to ensure that valves and fittings were not damaged and were able to maintain a sufficient vacuum before sampling. See Supporting Information for more details on the GSC preparation procedure.

Following the return of the gas samples to the Environmental Chemistry Laboratory, each canister's sample pressure was measured. This initial pressure and the dosing information provided the calibration for each canister. Subsequent GC/MS analyses quantitated the recovery of each of the compounds. The VOC analyses were based on EPA Method TO-15A, which was modified to accommodate constraints related to spaceflight operations. See Supporting Information for a complete description of the trace gas analysis method.

Results

The analyses generated a large dataset whose raw results (reported in mg/m^3) are provided in the Supporting Information. A total of 93 compounds were evaluated. Of these, 28 compounds were not observed in any of the samples (i.e., below the reporting limit) and are listed in Table 1 (all halogens). No fluorinated or brominated VOCs were detected. Additionally, few chlorinated compounds were observed beyond mono-substituted species.

Of the polychlorides, only 1,2-dichloroethane and 1,1,2,2-tetrachloroethane were observed in any of the samples, with the latter observed in the reactor gases of only one of the post-flight triplicates (0.2 mg/m^3), and the former in all three of the post-flight reactor samples (0.44, 0.28, and 0.41 mg/m^3). Chlorinated compounds that were observed included chloromethane, vinyl chloride, chloroethane, and 3-chloropropene. Therefore, it appears that the combustion process/waste simulant used here does not produce a significant amount of polychlorides. This is not surprising since chlorine represents only 0.11% by mass of the waste simulant.

For easier comparison between the lab and flight tests, the 63 observed compounds were categorized into groups: carbonyls, other carbohydrates (i.e., CHO), aromatic hydrocarbons, aromatic halogens, furans and dioxins, aliphatic hydrocarbons, nitrogen-containing (CHN) compounds, aliphatic halogens, thiols and sulfides, and siloxanes. To compare between tests, the total mass of each VOC was calculated from the pressure and volume of the pertinent collection tank/reactor and then normalized by the amount of trash combusted for each test (calculated from the differential dry mass of the trash before and after combustion). The resulting values are then reported

Table 2. Comparisons of flight VOCs to laboratory tests, reported in mg VOC/kg trash combusted. Cells shaded in blue denote chemical categories where the flight value falls outside of the 95% CI for the lab measurements.

	Collection Tank 2 (T2)		Collection Tank 3 (T3)		Reactor	
VOC Type	Flight	Lab Average	Flight	Lab Average	Flight	Lab Average
Carbonyls	1.42	0.28±0.32	1.40	0.39±0.05	666.2	684.6±113.2
Other CHO	--	--	0.06	--	193.6	57.9±53.3
Aromatic hydrocarbons	--	--	0.06	0.04	426.2	130.1±114.8
Aromatic halogens	--	--	--	--	--	0.9±1.2
Furans/dioxins	--	--	0.26	--	87.5	40.0±18.5
Aliphatic hydrocarbons	94.39	3.33±6.56	256.83	4.64±3.90	1088.2	281.2±123.5
CHN	--	0.04	0.10	0.02	22.9	12.6±21.5
Aliphatic halogens	1.76	0.20±0.30	6.27	0.48±0.27	20.8	11.8±7.8
Thiols/sulfides	2.73	1.18±0.99	4.26	0.86±0.13	8.3	6.2±11.2
Siloxanes	--	0.30	--	0.21	--	0.3
Total VOCs	100.30	5.09±6.97	269.24	6.48±4.04	2513.7	1225.4±274.7

in mg VOC/kg trash combusted and are shown in Table 2. Here, the lab average values include 95% confidence intervals (CIs). Where no intervals are provided, only a single lab trial was measured above the reporting limits; for these instances, the individual result is given. Cells shaded in blue denote chemical categories where the flight value falls outside of the 95% CI for the lab measurements.

The differences between the flight and laboratory tests are apparent. The flight results fall outside of the 95% CI for most of the VOC categories (where replicate measurements were observed), as well as for the total VOCs measured. Thus, VOC production from combustion in microgravity is statistically differentiable from combustion in a terrestrial laboratory. The compositions of the VOCs also vary, as shown in Figure 2.

Figure 2 shows important differences between terrestrial and microgravity combustion. Specifically, the microgravity VOC composition shown in Figure 2(A) favors the production of both aliphatic and aromatic hydrocarbons relative to the VOC composition from laboratory tests shown in Figure 2(B) (total of 60.25% for flight/microgravity versus 33.57% for lab tests). Furthermore, the microgravity combustion produced a lower fraction of carbonyls (26.50% for flight/microgravity versus 55.87% for the lab tests); indeed, carbonyls constitute the majority of the VOCs for lab tests.

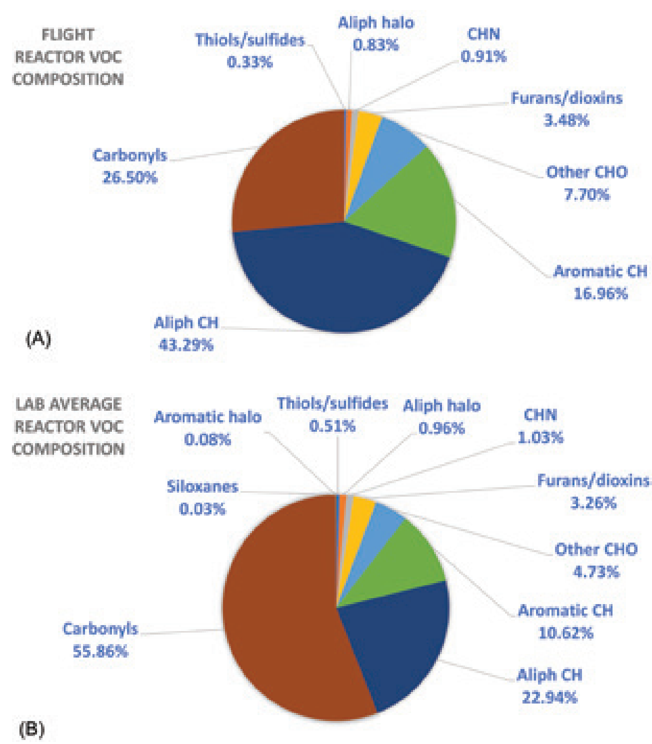

Figure 2. Comparison of VOC % mass compositions by category. **(A)** The composition of the VOCs observed in the flight reactor. **(B)** The average composition of the VOCs from the terrestrial laboratory analog tests.

Discussion

These results suggest that laboratory combustion was more efficient than for microgravity. The statistically significant larger mass of VOCs for the flight/microgravity test indicates that microgravity combustion was less complete. This agrees with the previously reported lower solid-to-gas conversion observed for the flight/microgravity test than for the laboratory tests (Pitts et al. 2022). Specifically, aliphatic and aromatic compounds represent fuels that combust to form CO_2 and water in an efficient system. Here, however,

Table 3. Individual SMAC Compound Comparisons in Reactor Gases. All values are given in ppm.

SMAC Compounds	Flight	Lab Avg	1-h SMAC	24-h SMAC	7-d SMAC	30-d SMAC	180-d SMAC
Propane	125.05	46.86±16.07	150	150	150	150	150
Vinyl chloride	0.89	0.12±0.19	130	30	1	1	1
Methanol	28.13	44.64±24.04	70	70	20	20	20
Acetaldehyde	350.65	299.89±116.69	10	6	2	2	2
Butane	79.00	18.77±13.86	18000	18000	18000	18000	18000
Ethanol	121.97	11.25±16.89	5000	5000	1000	1000	1000
Acrolein	1.19	51.61±8.88	0.075	0.035	0.015	0.015	0.008
Acetone	30.17	58.93±31.31	500	200	22	22	22
Propionaldehyde	26.28	53.52±90.32	45	45	5	5	5
Furan	27.46	17.73±14.21	4	0.4	0.025	0.025	0.025
Pentane	18.57	14.78±13.42	150	80	60	20	3
Isopropanol		9.87±40.99	400	100	60	60	60
Isoprene	6.83	0.08±0.06	50	25	2	2	1
t-Butanol		0.06±0.01	50	50	50	50	40
Butyraldehyde	13.82	25.79±24.82	45	45	5	5	5
Methyl ethyl ketone	12.71	12.61±5.15	50	50	10	10	10
Benzene	166.24	55.14±53.79	10	3	0.5	0.1	0.07
1-Butanol	1.21	0.72±1.25	50	25	25	25	12
Pentanal	13.69	12.86±5.27	45	45	5	5	5
n-Heptane	9.05	4.12±1.42	150	80	60	20	3
MIBK		0.75±1.20	35	35	35	35	35
Toluene	12.89	8.79±3.43	16	16	4	4	4
Octane	4.71	2.36±2.27	150	80	60	20	3
Hexanal	4.70	5.69±2.68	45	45	5	5	5
Ethylbenzene	1.45	1.04±1.13	180	60	30	30	12
m & p-Xylene	0.80	0.72±0.73	50	17	17	17	8.5
Nonane	1.68	1.13±1.73	150	80	60	20	3
Heptanal	2.08	2.76±3.96	45	45	5	5	5
o-Xylene	0.42	0.43±0.44	50	17	17	17	8.5
OMCTS	--	0.04	--	--	23	5	1

Flight value exceeds 95% CI. (blue shading) Flight value exceeds SMAC limit. (red shading)

it was observed that the flight/microgravity test left a larger fraction of these hydrocarbon compounds unreacted than the lab tests. Additionally, the higher composition of carbonyls (a combustion intermediate) for the lab tests shows a greater degree of oxidation than for microgravity. This corroborates reported comparisons between these tests, indicating a higher combustion efficiency (based on the CO_2:CO ratio) of the laboratory tests than the microgravity test (Meier et al. 2021). This also agrees with other reports of decreased combustion efficiency in microgravity due to the lack of buoyant convection (Cao et al. 2015; S. L. Olson 1991; Urban et al. 2019).

Of the 93 analyzed compounds, 37 of them appear on NASA's SMAC list (described above). Of those 37 SMAC compounds, 31 were observed in the OSCAR reactor either in the flight/microgravity test and/or in one or more of the laboratory tests. Table 3 lists the observed SMAC compounds and their reactor concentrations (in ppm), along with the SMAC concentrations for their different exposure durations.

The concentrations shaded in blue indicate SMAC compounds with microgravity concentrations outside of the 95% CI for the laboratory tests; in all but one of these cases (acrolein), the microgravity concentration was higher than the CI upper

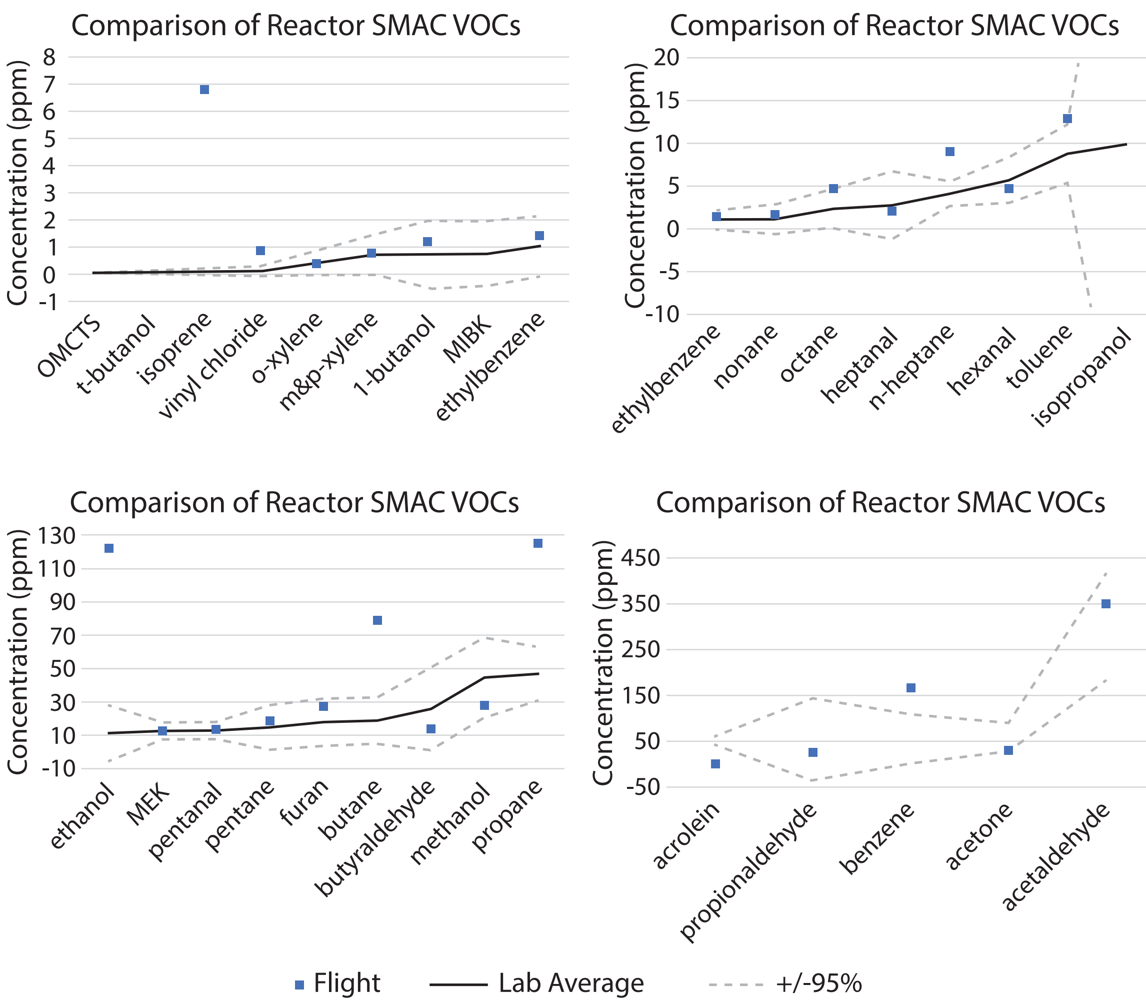

Figure 3. Plots of the flight/microgravity SMAC concentrations (blue squares) with the laboratory test average concentrations (black line) and the upper/lower boundaries of the 95% CI (gray dashed lines).

limit. This is consistent with the higher total VOC production observed for the flight/microgravity test. The lone exception is acrolein, whose flight/microgravity concentration was lower than the lower limit of the 95% CI for the lab tests (this is further discussed below). Figure 3 graphically represents these concentrations, with each plot displaying a successively higher concentration range.

Again, significant differences can be observed between the flight/microgravity test and the laboratory tests. Ten SMAC compounds for the flight/microgravity test fell outside of the 95% CI for the laboratory tests. These differences suggest that the VOC production for combustion in microgravity is significantly different than for terrestrial gravity.

Regarding the SMAC limits, concentrations in the reactor are critical quantities since they are higher than those in the collection tanks. A TtG system must be considered within the context of a transit vehicle. The current Mars mission architecture proposes a vehicle habitable volume of 116 m^3 (Ewert, Chen, and Powell, Camilah D. 2022). The authors' design considerations for a TtG reactor have a maximum volume of ~0.0165 m^3. Thus, for a worst-case critical failure scenario allowing the reactor gases to escape into the cabin, the volume ratio is 7,030:1. Table 4 shows the flight/microgravity SMAC concentrations as a percent of each SMAC limit before and after this dilution.

Both the undiluted (UD) reactor concentrations and the diluted (D) concentrations are included in the table. Where the result equals or exceeds the SMAC limit, the cell is shaded red. None of the diluted concentrations exceed the SMAC limits. The highest is furan at 110,000%, or ~1000-fold excess of its 180-day SMAC limit. But even for furan, dilution into the habitable volume results in 15.6% of the 180-day SMAC limit. Interestingly, acrolein was higher in concentration for laboratory tests (51.61±8.88 ppm) than for the flight test

Table 4. Observed reactor SMAC compounds from combustion of 10 g trash in microgravity as a percentage of the SMAC limit for exposures up to 180-days.

	% of 1-hour limit		% of 24-hour limit		% of 7-day limit		% of 30-day limit		% of 180-day limit	
SMAC Compound	**UD**	**D**	**UD**	**D**	**UD**	**D**	**UD**	**D**	**UD**	**D**
Propane	83.4	1.19e-2	83.4	1.19e-2	83.4	1.19e-2	83.4	1.19e-2	83.4	1.19e-2
Vinyl chloride	0.684	9.73e-5	2.96	4.21e-4	88.9	1.26e-2	88.9	1.26e-2	88.9	1.26e-2
Methanol	40.2	5.72e-3	40.2	5.72e-3	141	2.00e-2	141	2.00e-2	140	2.00e-2
Acetaldehyde	3.51e3	0.499	5.84e3	0.831	1.75e4	2.49	1.75e4	2.49	1.75e4	2.49
Butane	0.439	6.24e-5	0.439	6.24e-5	0.439	6.24e-5	0.439	6.24e-5	0.439	6.24e-5
Ethanol	2.44	3.47e-4	2.44	3.47e-4	12.2	1.73e-3	12.2	1.73e-3	12.2	1.73e-3
Acrolein	1.59e3	0.227	3.41e3	0.485	7.96e3	1.13	7.96e3	1.13	1.49e4	2.12
Acetone	6.03	8.58e-4	15.1	2.15e-3	137	1.95e-2	137	1.95e-2	137	1.95e-2
Propionaldehyde	58.4	8.31e-3	58.4	8.31e-3	526	7.48e-2	526	7.48e-2	526	7.48e-2
Furan	6.87e2	9.77e-2	6.87e3	0.977	1.10e5	15.6	1.10e5	15.6	1.10e5	15.6
Pentane	12.4	1.76e-3	23.2	3.30e-3	31.0	4.40e-3	92.8	1.32e-2	619	8.80e-2
Isoprene	13.7	1.94e-3	27.3	3.89e-3	342	4.86e-2	342	4.86e-2	683	9.72e-2
Butyraldehyde	30.7	4.37e-3	30.7	4.37e-3	276	3.93e-2	276	3.93e-2	276	3.93e-2
MEK	25.4	3.62e-3	25.4	3.62e-3	127	1.81e-2	127	1.81e-2	127	1.81e-2
Benzene	1.66e3	0.236	5.54e3	0.788	3.32e4	4.73	1.66e5	23.6	2.37e5	3.38
1-Butanol	2.42	3.45e-4	4.84	6.89e-4	4.84	6.89e-4	4.84	6.89e-4	10.1	1.44e-3
Pentanal	30.4	4.33e-3	30.4	4.33e-3	274	3.90e-2	274	3.90e-2	274	3.90e-2
n-Heptane	6.03	8.58e-4	11.3	1.61e-3	15.1	2.15e-3	45.3	6.44e-3	302	4.29e-2
Toluene	80.6	1.15e-2	80.6	1.15e-2	322	4.58e-2	322	4.58e-2	322	4.58e-2
Octane	3.14	4.47e-4	5.89	8.38e-4	7.86	1.12e-3	23.6	3.35e-3	157	2.23e-2
Hexanal	10.5	1.49e-3	10.5	1.49e-3	94.0	1.34e-2	94.0	1.34e-2	94.0	1.34e-2
Ethylbenzene	0.803	1.14e-4	2.41	3.43e-4	4.82	6.86e-4	4.82	6.86e-4	12.1	1.71e-3
m & p-Xylene	1.60	2.27e-4	4.70	6.68e-4	4.70	6.68e-4	4.70	6.68e-4	9.40	1.34e-3
Nonane	1.12	1.59e-4	2.10	2.98e-4	2.80	3.98e-4	8.39	1.19e-3	55.9	7.95e-3
Heptanal	4.62	6.57e-4	4.62	6.57e-4	41.6	5.91e-3	41.6	5.91e-3	41.6	5.91e-3
o-Xylene	0.832	1.18e-4	2.45	3.48e-4	2.45	3.48e-4	2.45	3.48e-4	4.89	6.96e-4

UD = percentage based on the undiluted reactor concentration. D = percentage based on the diluted concentration into a transit vehicle's habitable volume. Results ≥ 100% are shaded red.

(1.19 ppm). Acrolein is a carbonyl that has been reported to be a product of the oxidation of aliphatic species as well as complex materials (Sun et al. 2023; Hartikainen et al. 2018; Shields et al. 1995; Terrill, Montgomery, and Reinhardt 1978; Einhorn 1975). The SMAC limits for acrolein are shown in Table 3. For the lab tests, undiluted percentages for acrolein are 68,800%, 147,000%, 344,000%, 344,000%, and 645,000%, and diluted percentages are 9.8%, 20.9%, 48.9%, 48.9%, and 91.7%, for the respective durations. These are the highest values for all of the SMAC compounds observed. Thus, acrolein represents an important hazard, especially as microgravity TtG reactors are developed with higher efficiencies.

Conclusions

The primary conclusion here is that the difference in VOC production between combustion in microgravity versus terrestrial gravity is significant. There was a statistically significant higher VOC production for microgravity than for the laboratory tests. Indeed, for total VOCs, the flight values fell outside the 95% CI by as much as 32 times the range of the CI from the lab test averages. While this corroborates the previously reported observation that the flight test showed a decreased ratio of CO_2:CO versus the lab tests, the statistical treatment of the CO_2:CO ratio was not definitive.(Pitts et al.

2022) In that case, the values for the microgravity test fell just within the 95% CI for the three laboratory results; thus, the null hypothesis (that the measurements are not differentiable) could not be rejected. In the case of VOCs, however, the rejection of the null hypothesis was quite definitive, indicating a statistically significant difference between the combustion of trash in microgravity versus terrestrial gravity.

The reason for this difference is less apparent. While the flight test was very successful, there was one important anomaly. Namely, there was a coarse steel wire mesh in the reactor meant to hold the trash near the bottom (as for laboratory tests) that moved during flight due to the vibrations associated with the launch. As a result, under microgravity, the trash migrated into a larger volume within the reactor. Laboratory tests with the mesh in different positions revealed a strong dependence of the combustion efficiency (via the CO_2:CO ratio) on the mesh position. For laboratory tests with the mesh partially raised to the height observed during the flight (measured from the flight reactor video), a larger CO_2:CO ratio was observed (26.1:1 for the lab test versus 12.0:1 for flight) (Pitts et al. 2022). Furthermore, lab tests with the mesh fully raised (to the top of the reactor) showed a ratio of 77.5:1, corresponding to more efficient combustion and suggesting that the mesh is a flame and heat barrier. However, trace gas analyses were performed only for the 'fully raised mesh' laboratory tests (at the time understood to be the position of the mesh during the flight) corresponding to more efficient combustion. Note that correlations with combustion efficiencies and CO_2:CO ratios have been reported for numerous fuel types (Matthes and Hartmann 2017; Gopan et al. 2017; Chien, Escofet-Martin, and Dunn-Rankin 2016; Svoboda et al. 2009; Wallington, Kaiser, and Farrell 2006; Lee et al. 2005; Johansson et al. 2004; Cliffe and Patumsawad 2001; Hasselriis, Floyd 1992). In any case, it is apparent that combustion in microgravity is less efficient than in an equivalent terrestrial arrangement. Furthermore, the raised mesh/larger volume of the flight test is an important result since it more closely approximates a likely reactor scenario for a full-scale system.

The SMAC list is not exhaustive regarding harmful compounds, especially considering the myriad VOCs present in a combustion effluent. If thermal processes are used to process trash on spacecraft, a more comprehensive appraisal of the potential hazards in the effluent gases will be required. Additionally, the SMAC list includes hazardous species that were not analyzed here and should be evaluated in future work.

While a final reactor design should protect against leaks into a spacecraft's habitable volume, this study suggests that the resulting dilution should provide some protection even in the event of a catastrophic failure; however, it must be noted that VOC concentrations in a full-scale reactor might be higher than for the sub-scale OSCAR reactor. Additionally, hazardous VOCs could be reduced by effective filtering/sequestering and/or other abatement methods, such as reducing VOCs in a plasma system. It is likely that a final TtG system will include multiple abatement systems. Indeed, abatement systems (such as plasma) might be used to produce commodities as feedstocks for other systems. These results provide a foundational basis from which to evaluate the performance of such VOC abatement systems.

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Supporting Information

Grab Sample Container procedure for leak checking, cleaning, proofing, evacuating, and dosing.

A 96-hour leak check was performed on each canister at a pressure of 4 mTorr. After completion of a successful 96-hour leak test, the GSCs underwent an internal cleaning procedure, which included multiple heating (100 °C) and purging/evacuation cycles with humidified nitrogen (UHP-grade) to remove potential contaminants. After cleaning, the GSCs were filled to approximately 10 psig using humidified zero air. The canisters were then 'proofed' to ensure that they were free of analyte contaminants. The proofing process involved the analyses of the canister air samples for approximately 100 target VOCs by gas chromatography/mass spectrometry (GC/MS). A canister was considered clean if all target VOCs were measured to be ≤5 ppbv, with one exception being acetaldehyde, which was required to measure ≤10 ppbv. Proofed canisters were reattached to the vacuum manifold and evacuated to 4 mTorr prior to dosing with a gas-phase surrogate mixture.

A gas-phase surrogate stock standard dosing mixture was prepared in a 6L canister. This dosing mixture contained three compounds, including acetone-C13, chlorobenzene-d5, and fluorobenzene-d5, not typically found in ambient or process air samples, and was used for reference purposes only. A gas-tight syringe was used to add a small amount of dosing mixture to each canister. Following the dosing, preparation of the canisters was complete.

Trace Gas Analysis Method

Prior to the beginning of sample analysis, the initial pressure of the GSC was measured. Samples were then pressurized with ultra-high-purity nitrogen at an ambient pressure that was higher than the necessary pressure to ensure adequate sample volume.

The analyses included concentrating the VOCs and then separating the mixtures into their components for subsequent identification and quantitation. This process was accomplished by introducing samples into an integrated analytical system consisting of an automated inlet system (AIS), a gas chromatograph (GC), a mass selective detector (MSD), and a data system (DS). The GSC was first connected to an automated inlet device containing a series of traps for the management of water and carbon dioxide present in the samples. Following water and carbon dioxide management, the concentrated sample was refocused using liquid nitrogen to achieve a better signal in the chromatograph and then injected into the GC capillary column, where the sample components were separated and resolved. Resolved sample components were then transferred into an MSD operating in the SCAN mode where their specific electronic signatures (mass spectra) were stored for subsequent identification and quantification.

In order for the sample measurements to be within the ranges of the calibration curves, the GC injection volumes were adjusted accordingly and/or the gas samples were pressure diluted with zero air. These changes were quantitatively accounted for by analyses of the dosing compounds (see above). This also is the reason that the reporting limits vary for the same analyte from different gas samples (see Supporting Information for analyte reporting limits).

Acceptance limits for quality control checks were defined in the work instruction. When quality control criteria could not be achieved, corrective action and troubleshooting of instrumentation was required and documented.

During canister preparation, a minimum of one laboratory control was prepared for every ten GSCs dosed. After sample canisters were received by the Environmental Chemistry Laboratory, the canisters were logged into a sample login folder and laboratory tracking numbers were generated. For sample analysis, instrumentation was demonstrated to be linear over a wide range of concentrations and determined to be stable as shown by daily calibration verifications using standard mixtures. To assess the accuracy of sampling and the GC/MS analysis process, air samples were measured as the percent recovery of three surrogates spiked in the GSCs during pre-sampling preparation. These results were compared to laboratory surrogate controls, prepared during both pre-sampling and post-sampling processing. Finally, analytical results were verified by use of an independent computer calculation routine, and the Internal Quality Representative (IQR) conferred with analytical chemists, when necessary, to ensure that all data generated were scientifically sound and of adequately known precision and accuracy. All documentation was maintained by the IQR in electronic form in the Environmental Chemistry Laboratory.

Results of TO-15 analyses.

All values are listed in units of mg/m^3.

* Quantified using a multi-point calibration

< : Value is less than the laboratory reporting limit (shown).

T1 = gases from Tank T1 (this was not reported in the manuscript; T1 was collected as a control before combustion was initiated).

T2 = gases from Tank T2
T3 = gases from Tank T3
R = gases from the Reactor
rm = gases from ambient room air collected as a control
Flight = gases collected from the flight experiment
Lab X = gases collected from laboratory experiment trial X

Target Compounds (TO-15)*	Flight T3	Flight T1	Flight T2	Flight rm	Flight R
1,1,1,2-Tetrafluoroethane	<0.083	<0.12	<0.083	<0.031	<2.5
Perfluoro(2-methylpentane)	<0.17	<0.23	<0.17	<0.062	<4.9
Propene	98.86	1.1	38.33	<0.0077	214.03
Propane	108.44	0.16	41.99	<0.0081	222.37
Carbonyl sulfide (Carbon oxide sulfide)	0.78	<0.041	0.63	<0.011	3.7
Freon 12 (Dichlorodifluoromethane)	<0.059	<0.083	<0.059	<0.022	<1.7
Chloromethane	7.02	<0.035	1.69	<0.0093	21.09
Freon 114 (1,2-Dichloro-1,1,2,2-tetrafluoroethane)	<0.084	<0.12	<0.084	<0.031	<2.5
Isobutane	2.1	<0.040	0.49	<0.011	4.97
Vinyl chloride	1.57	<0.043	0.29	<0.012	2.24
Methanol	0.09	<0.037	<0.026	0.06	36.34
Acetaldehyde	0.24	2.34	1.28	0.09	622.83
2-Methyl-1-propene	112.56	0.16	19.59	<0.010	486.87
Butane	29.18	0.05	5.19	<0.011	185.13
1,3-Butadiene	0.56	0.06	0.06	<0.0100	217.79
Bromomethane	<0.047	<0.065	<0.047	<0.017	<1.4
Chloroethane	0.1	<0.044	<0.032	<0.012	5.48
Ethanol	<0.023	0.1	<0.023	1.76	226.57
Freon 11 (Trichlorofluoromethane)	<0.067	<0.094	<0.067	<0.025	<2.0
Propenal (Acrolein)	0.59	<0.039	0.08	<0.010	2.7
Acetonitrile	0.14	<0.028	<0.020	<0.0076	16.34
Acetone	0.53	0.29	0.14	0.12	70.66
Propanal (Propionaldehyde)	0.45	0.04	0.1	0.02	61.54
Furan	0.36	<0.047	<0.033	<0.013	75.38
Pentane	4.1	<0.050	0.56	<0.013	54.02
2-Propanol (Isopropanol)	<0.049	0.44	<0.049	0.4	<1.4
Isoprene (2-Methyl-1,3-butadiene)	<0.033	<0.047	<0.033	<0.013	18.77
1,1-Dichloroethene	<0.048	<0.067	<0.048	<0.018	<1.4
Dimethyl sulfide	<0.030	<0.043	<0.030	<0.011	1.18
Acrylonitrile	<0.026	<0.036	<0.026	<0.0098	15.4
Freon 113 (1,1,2-Trichloro-1,2,2-trifluoroethane)	<0.092	<0.13	<0.092	<0.034	<2.7
2-Methyl-2-propanol	<0.036	<0.051	<0.036	<0.014	<1.1
Methyl acetate	<0.036	<0.051	<0.036	<0.014	1.58
3-Chloropropene (Allyl chloride)	<0.038	<0.053	<0.038	<0.014	<1.1

Target Compounds (TO-15)*	Flight T3	Flight T1	Flight T2	Flight rm	Flight R
Methylene chloride (Dichloromethane)	<0.042	<0.058	<0.042	<0.016	<1.2
Carbon disulfide	5.12	<0.052	2.44	<0.014	6.69
1-Propanol	<0.029	<0.041	<0.029	<0.011	1.79
Trimethylsilanol	<0.044	<0.062	<0.044	<0.017	<1.3
1,1-Dichloroethane	<0.049	<0.068	<0.049	<0.018	<1.4
Butanal (Butyraldehyde)	0.05	<0.050	<0.035	0.01	40.18
2-Butanone (Methyl ethyl ketone)	<0.035	<0.050	<0.035	<0.013	36.97
Hexane	0.18	<0.059	<0.042	<0.016	37.39
2-Methylfuran	<0.040	<0.056	<0.040	<0.015	35.21
cis-1,2-Dichloroethene	<0.048	<0.067	<0.048	<0.018	<1.4
Ethyl acetate	<0.043	<0.061	<0.043	<0.016	<1.3
Chloroform	<0.059	<0.082	<0.059	<0.022	<1.7
1,1,1-Trichloroethane	<0.065	<0.092	<0.065	<0.025	<1.9
2-Butenal	0.08	<0.048	<0.034	<0.013	<1.0
1,2-Dichloroethane	<0.049	<0.068	<0.049	<0.018	<1.4
Benzene	0.09	<0.054	<0.038	<0.014	523.59
Carbon tetrachloride	<0.075	<0.11	<0.075	<0.028	<2.2
1-Butanol	<0.036	<0.051	<0.036	<0.014	3.62
2-Methylhexane	<0.049	<0.069	<0.049	<0.018	<1.4
2,3-Dimethylpentane	<0.049	<0.069	<0.049	<0.018	<1.4
3-Methylhexane	<0.049	<0.069	<0.049	<0.018	<1.4
2-Pentanone	<0.042	<0.059	<0.042	<0.016	10.85
Pentanal	<0.042	<0.059	<0.042	<0.016	47.56
n-Heptane	<0.049	<0.069	<0.049	<0.018	36.57
Trichloroethene	<0.064	<0.090	<0.064	<0.024	<1.9
1,2-Dichloropropane	<0.055	<0.078	<0.055	<0.021	<1.6
2,5-Dimethylfuran	<0.047	<0.066	<0.047	<0.018	10.65
1,4-Dioxane	<0.043	<0.061	<0.043	<0.016	<1.3
4-Methyl-2-pentanone (MIBK)	<0.049	<0.069	<0.049	<0.018	<1.4
cis-1,3-Dichloropropene	<0.054	<0.076	<0.054	<0.020	<1.6
2-Pentenal	<0.041	<0.058	<0.041	<0.015	<1.2
trans-1,3-Dichloropropene	<0.054	<0.076	<0.054	<0.020	<1.6
Toluene	<0.045	<0.063	<0.045	<0.017	47.9
1,1,2-Trichloroethane	<0.065	<0.092	<0.065	<0.025	<1.9
Mesityl oxide (4-Methyl-3-penten-2-one)	<0.048	<0.067	<0.048	<0.018	<1.4
Octane	<0.056	<0.078	<0.056	<0.021	21.71
Hexanal	<0.049	<0.069	<0.049	0.03	18.99
Butyl acetate	<0.057	<0.080	<0.057	<0.021	<1.7
Tetrachloroethene (Perchloroethene)	<0.081	<0.11	<0.081	<0.031	<2.4
1,2-Dibromoethane (EDB)	<0.092	<0.13	<0.092	<0.035	<2.7
Chlorobenzene	<0.055	<0.077	<0.055	<0.021	<1.6
Ethylbenzene	<0.055	<0.077	<0.052	<0.020	6.19

Target Compounds (TO-15)*	Flight T3	Flight T1	Flight T2	Flight rm	Flight R
m & p-Xylene	<0.010	<0.015	<0.10	<0.039	3.42
2-Heptanone	<0.056	<0.078	<0.056	<0.021	<1.6
Nonane	<0.063	<0.088	<0.063	<0.024	8.67
Styrene (Ethenylbenzene)	<0.051	<0.072	<0.051	<0.019	7.9
Heptanal	<0.056	<0.078	<0.056	<0.021	9.57
o-Xylene	<0.052	<0.073	<0.052	<0.020	1.78
Cyclohexanone	<0.048	<0.067	<0.048	<0.018	<1.4
1,1,2,2-Tetrachloroethane	<0.082	<0.012	<0.082	<0.031	<2.4
Octamethylcyclotetrasiloxane (OMCTS)	<0.24	<0.34	<0.24	<0.091	<7.1
1,3,5-Trimethylbenzene	<0.059	<0.083	<0.059	<0.022	<1.7
1,2,4-Trimethylbenzene	<0.059	<0.083	<0.059	<0.022	<1.7
1,3-Dichlorobenzene	<0.072	<0.10	<0.072	<0.027	<2.1
1,4-Dichlorobenzene	<0.072	<0.10	<0.072	<0.027	<2.1
1,2-Dichlorobenzene	<0.072	<0.10	<0.072	<0.027	<2.1
Decamethylcyclopentasiloxane (DMCPS)	<0.30	<0.42	<0.30	<0.11	<8.9
1,2,4-Trichlorobenzene	<0.15	<0.21	<0.15	<0.056	<4.4
Hexachlorobutadiene	<0.13	<0.18	<0.13	<0.048	<3.8

Target Compounds (TO-15)*	Lab 1 T1	Lab 1 T2	Lab 1 T3	Lab 1 R	Lab 2 T2
1,1,1,2-Tetrafluoroethane	<0.10	<0.083	<0.083	<0.13	<0.083
Perfluoro(2-methylpentane)	<0.21	<0.17	<0.17	<0.25	<0.17
Propene	0.2	1.8	3.58	93	7.46
Propane	0.04	0.39	0.68	95	0.59
Carbonyl sulfide (Carbon oxide sulfide)	<0.037	0.61	0.69	1.3	1.3
Freon 12 (Dichlorodifluoromethane)	<0.074	<0.059	<0.059	<0.089	<0.059
Chloromethane	<0.031	0.08	0.53	8.3	0.31
Freon 114 (1,2-Dichloro-1,1,2,2-tetrafluoroethane)	<0.10	<0.084	<0.084	<0.13	<0.084
Isobutane	<0.036	<0.029	<0.029	3.6	<0.029
Vinyl chloride	<0.038	<0.031	0.12	0.17	0.061
Methanol	<0.033	<0.026	<0.026	70	<0.026
Acetaldehyde	0.14	0.16	0.37	497	0.19
2-Methyl-1-propene	0.04	0.17	0.67	203	0.19
Butane	<0.036	0.12	0.28	35	0.11
1,3-Butadiene	<0.033	<0.027	<0.027	17	<0.027
Bromomethane	<0.058	<0.047	<0.047	<0.070	<0.047
Chloroethane	<0.040	<0.032	<0.032	5.1	<0.032
Ethanol	<0.028	<0.023	<0.023	12.3	<0.023
Freon 11 (Trichlorofluoromethane)	<0.084	<0.067	<0.067	<0.10	<0.067
Propenal (Acrolein)	<0.034	<0.028	<0.028	112	<0.028
Acetonitrile	<0.025	<0.020	0.03	7.9	<0.020
Acetone	0.14	0.06	0.14	168	0.08
Propanal (Propionaldehyde)	<0.036	<0.029	0.052	186	<0.029

Target Compounds (TO-15)*	Lab 1 T1	Lab 1 T2	Lab 1 T3	Lab 1 R	Lab 2 T2
Furan	<0.042	<0.033	<0.033	31	<0.033
Pentane	<0.044	<0.035	0.04	29	<0.035
2-Propanol (Isopropanol)	<0.061	<0.049	<0.049	0.83	<0.049
Isoprene (2-Methyl-1,3-butadiene)	<0.042	<0.033	<0.033	0.17	<0.033
1,1-Dichloroethene	<0.059	<0.048	<0.048	<0.071	<0.048
Dimethyl sulfide	<0.038	<0.030	<0.030	0.97	<0.030
Acrylonitrile	<0.033	<0.026	<0.026	8.5	<0.026
Freon 113 (1,1,2-Trichloro-1,2,2-trifluoro-ethane)	<0.11	<0.092	<0.092	<0.14	<0.092
2-Methyl-2-propanol	<0.045	<0.036	<0.036	0.19	<0.036
Methyl acetate	<0.045	<0.036	<0.036	1.3	<0.036
3-Chloropropene (Allyl chloride)	<0.047	<0.038	<0.038	0.18	<0.038
Methylene chloride (Dichloromethane)	<0.052	<0.042	<0.042	<0.063	<0.042
Carbon disulfide	<0.047	0.31	0.71	4.7	0.49
1-Propanol	<0.037	<0.029	<0.029	2.41	<0.029
Trimethylsilanol	<0.055	<0.044	<0.044	<0.066	<0.044
1,1-Dichloroethane	<0.061	<0.049	<0.049	<0.073	<0.049
Butanal (Butyraldehyde)	<0.044	<0.035	0.036	45	0.04
2-Butanone (Methyl ethyl ketone)	<0.044	<0.035	0.054	31	<0.035
Hexane	<0.053	<0.042	<0.042	17	<0.042
2-Methylfuran	<0.050	<0.040	<0.040	16	<0.040
cis-1,2-Dichloroethene	<0.059	<0.048	<0.048	<0.071	<0.048
Ethyl acetate	<0.054	<0.043	<0.043	<0.065	<0.043
Chloroform	<0.073	<0.059	<0.059	<0.088	<0.059
1,1,1-Trichloroethane	<0.082	<0.065	<0.065	<0.098	<0.065
2-Butenal	<0.043	<0.034	<0.034	7.2	<0.034
1,2-Dichloroethane	<0.061	<0.049	<0.049	0.44	<0.049
Benzene	<0.048	<0.038	<0.038	216	<0.038
Carbon tetrachloride	<0.094	<0.075	<0.075	<0.11	<0.075
1-Butanol	<0.045	<0.036	<0.036	3.9	<0.036
2-Methylhexane	<0.061	<0.049	<0.049	0.29	<0.049
2,3-Dimethylpentane	<0.061	<0.049	<0.049	0.41	<0.049
3-Methylhexane	<0.061	<0.049	<0.049	<0.074	<0.049
2-Pentanone	<0.053	<0.042	<0.042	18	<0.042
Pentanal	<0.053	<0.042	<0.042	42	<0.042
n-Heptane	<0.061	<0.049	<0.049	18	<0.049
Trichloroethene	<0.081	<0.064	<0.064	<0.097	<0.064
1,2-Dichloropropane	<0.069	<0.055	<0.055	<0.083	<0.055
2,5-Dimethylfuran	<0.059	<0.047	<0.047	5.4	<0.047
1,4-Dioxane	<0.054	<0.043	<0.043	0.87	<0.043
4-Methyl-2-pentanone (MIBK)	<0.061	<0.049	<0.049	3	<0.049
cis-1,3-Dichloropropene	<0.068	<0.054	<0.054	<0.082	<0.054
2-Pentenal	<0.052	<0.041	<0.041	6.7	<0.041

Target Compounds (TO-15)*	Lab 1 T1	Lab 1 T2	Lab 1 T3	Lab 1 R	Lab 2 T2
trans-1,3-Dichloropropene	<0.068	<0.054	<0.054	<0.082	<0.054
Toluene	<0.057	<0.045	<0.045	34	<0.045
1,1,2-Trichloroethane	<0.082	<0.065	<0.065	<0.098	<0.065
Mesityl oxide (4-Methyl-3-penten-2-one)	<0.060	<0.048	<0.048	3.1	<0.048
Octane	<0.070	<0.056	<0.056	15	<0.056
Hexanal	<0.061	<0.049	<0.049	26	<0.049
Butyl acetate	<0.071	<0.057	<0.057	<0.086	<0.057
Tetrachloroethene (Perchloroethene)	<0.10	<0.081	<0.081	<0.12	<0.081
1,2-Dibromoethane (EDB)	<0.12	<0.092	<0.092	<0.14	<0.092
Chlorobenzene	<0.069	<0.055	<0.055	0.31	<0.055
Ethylbenzene	<0.065	<0.052	<0.052	6.7	<0.052
m & p-Xylene	<0.13	<0.10	<0.10	4.5	<0.10
2-Heptanone	<0.070	<0.056	<0.056	3.1	<0.056
Nonane	<0.079	<0.063	<0.063	10	<0.063
Styrene (Ethenylbenzene)	<0.064	<0.051	<0.051	4.8	<0.051
Heptanal	<0.070	<0.056	<0.056	21	<0.056
o-Xylene	<0.065	<0.052	<0.052	2.7	<0.052
Cyclohexanone	<0.060	<0.048	<0.048	1.4	<0.048
1,1,2,2-Tetrachloroethane	<0.10	<0.082	<0.082	0.2	<0.082
Octamethylcyclotetrasiloxane (OMCTS)	<0.30	<0.24	0.35	0.52	0.43
1,3,5-Trimethylbenzene	<0.074	<0.059	<0.059	1	<0.059
1,2,4-Trimethylbenzene	<0.074	<0.059	<0.059	0.57	<0.059
1,3-Dichlorobenzene	<0.090	<0.072	<0.072	<0.11	<0.072
1,4-Dichlorobenzene	<0.090	<0.072	<0.072	<0.11	<0.072
1,2-Dichlorobenzene	<0.090	<0.072	<0.072	<0.11	<0.072
Decamethylcyclopentasiloxane (DMCPS)	<0.38	<0.30	<0.30	<0.45	<0.30
1,2,4-Trichlorobenzene	<0.19	<0.15	<0.15	<0.22	<0.15
Hexachlorobutadiene	<0.16	<0.13	<0.13	<0.19	<0.13

Target Compounds (TO-15)*	Lab 2 T3	Lab 2 R	Lab 2 rm	Lab 3 T1	Lab 3 T2
1,1,1,2-Tetrafluoroethane	<0.10	<0.15	<0.027	<0.12	<0.10
Perfluoro(2-methylpentane)	<0.21	<0.29	<0.054	<0.24	<0.21
Propene	9.05	71	0.014	0.036	0.71
Propane	<0.027	72	<0.0070	<0.031	1
Carbonyl sulfide (Carbon oxide sulfide)	0.91	1.7	<0.0096	<0.043	1.6
Freon 12 (Dichlorodifluoromethane)	<0.074	<0.10	<0.019	<0.086	<0.074
Chloromethane	0.81	9.4	<0.0081	<0.036	0.26
Freon 114 (1,2-Dichloro-1,1,2,2-tetrafluoroethane)	<0.10	<0.15	<0.027	<0.12	<0.10
Isobutane	0.038	1.2	<0.0093	<0.041	<0.036
Vinyl chloride	0.24	0.19	<0.0100	<0.044	0.083
Methanol	<0.033	58	0.011	0.088	<0.033
Acetaldehyde	0.43	473	0.02	0.42	0.2

Target Compounds (TO-15)*	Lab 2 T3	Lab 2 R	Lab 2 rm	Lab 3 T1	Lab 3 T2
2-Methyl-1-propene	1.2	184	<0.0090	<0.040	0.3
Butane	0.59	59	<0.0093	<0.041	0.2
1,3-Butadiene	<0.033	11	<0.0086	<0.038	<0.033
Bromomethane	<0.058	<0.082	<0.015	<0.068	<0.058
Chloroethane	<0.040	9.9	<0.010	<0.046	<0.040
Ethanol	<0.028	35.4	<0.0073	<0.033	<0.028
Freon 11 (Trichlorofluoromethane)	<0.084	<0.12	<0.022	<0.098	<0.084
Propenal (Acrolein)	<0.034	112	<0.0089	0.092	<0.034
Acetonitrile	<0.025	14	<0.0065	0.079	0.05
Acetone	0.15	137	0.04	0.46	0.17
Propanal (Propionaldehyde)	0.074	162	<0.0093	0.15	0.045
Furan	<0.042	54	<0.011	<0.048	<0.042
Pentane	0.066	40	<0.012	<0.051	<0.044
2-Propanol (Isopropanol)	<0.061	47	0.12	<0.071	<0.061
Isoprene (2-Methyl-1,3-butadiene)	<0.042	<0.059	<0.011	<0.048	<0.042
1,1-Dichloroethene	<0.059	<0.083	<0.015	<0.069	<0.059
Dimethyl sulfide	<0.038	0.7	<0.0099	<0.044	<0.038
Acrylonitrile	<0.033	25	<0.0085	0.055	<0.033
Freon 113 (1,1,2-Trichloro-1,2,2-trifluoro-ethane)	<0.11	<0.16	<0.030	<0.13	<0.11
2-Methyl-2-propanol	<0.045	<0.064	<0.012	<0.053	<0.045
Methyl acetate	<0.045	0.72	<0.012	<0.053	<0.045
3-Chloropropene (Allyl chloride)	<0.047	0.15	<0.012	<0.054	<0.047
Methylene chloride (Dichloromethane)	<0.052	<0.073	<0.014	<0.060	<0.052
Carbon disulfide	0.7	2.8	<0.012	<0.054	0.32
1-Propanol	<0.037	<0.052	<0.0096	<0.043	<0.037
Trimethylsilanol	<0.055	<0.077	<0.014	0.06	<0.055
1,1-Dichloroethane	<0.061	<0.085	<0.016	<0.070	<0.061
Butanal (Butyraldehyde)	<0.044	77	<0.012	0.078	<0.044
2-Butanone (Methyl ethyl ketone)	<0.044	43	<0.012	0.11	<0.044
Hexane	<0.053	16	<0.014	<0.061	<0.053
2-Methylfuran	<0.050	13	<0.013	<0.058	<0.050
cis-1,2-Dichloroethene	<0.059	<0.083	<0.015	<0.069	<0.059
Ethyl acetate	<0.054	<0.076	<0.014	<0.063	<0.054
Chloroform	<0.073	<0.10	<0.019	<0.085	<0.073
1,1,1-Trichloroethane	<0.082	<0.11	<0.021	<0.095	<0.082
2-Butenal	<0.043	8.2	<0.011	0.068	<0.043
1,2-Dichloroethane	<0.061	0.28	<0.016	<0.070	<0.061
Benzene	0.066	210	<0.012	0.17	<0.048
Carbon tetrachloride	<0.094	<0.13	<0.025	<0.11	<0.094
1-Butanol	<0.045	1.2	<0.012	<0.053	<0.045
2-Methylhexane	<0.061	<0.086	<0.016	<0.071	<0.061
2,3-Dimethylpentane	<0.061	<0.086	<0.016	<0.071	<0.061

Target Compounds (TO-15)*	Lab 2 T3	Lab 2 R	Lab 2 rm	Lab 3 T1	Lab 3 T2
3-Methylhexane	<0.061	<0.086	<0.016	<0.071	<0.061
2-Pentanone	<0.053	13	<0.014	0.11	<0.053
Pentanal	<0.053	53	<0.014	0.14	<0.053
n-Heptane	<0.061	18	<0.016	<0.071	<0.061
Trichloroethene	<0.081	<0.11	<0.021	<0.094	<0.081
1,2-Dichloropropane	<0.069	<0.097	<0.018	<0.080	<0.069
2,5-Dimethylfuran	<0.059	1.4	<0.015	<0.068	<0.059
1,4-Dioxane	<0.054	0.21	<0.014	<0.063	<0.054
4-Methyl-2-pentanone (MIBK)	<0.061	1.1	<0.016	<0.071	<0.061
cis-1,3-Dichloropropene	<0.068	<0.095	<0.018	<0.079	<0.068
2-Pentenal	<0.052	2.8	<0.013	<0.060	<0.052
trans-1,3-Dichloropropene	<0.068	<0.095	<0.018	<0.079	<0.068
Toluene	<0.057	37	<0.015	<0.066	<0.057
1,1,2-Trichloroethane	<0.082	<0.11	<0.021	<0.095	<0.082
Mesityl oxide (4-Methyl-3-penten-2-one)	<0.060	<0.084	<0.016	<0.070	<0.060
Octane	<0.070	11	<0.018	<0.081	<0.070
Hexanal	<0.061	25	<0.016	0.12	<0.061
Butyl acetate	<0.071	<0.10	<0.019	<0.083	<0.071
Tetrachloroethene (Perchloroethene)	<0.10	<0.14	<0.026	<0.12	<0.10
1,2-Dibromoethane (EDB)	<0.12	<0.16	<0.030	<0.13	<0.12
Chlorobenzene	<0.069	0.15	<0.018	<0.080	<0.069
Ethylbenzene	<0.065	3.5	<0.017	<0.076	<0.065
m & p-Xylene	<0.13	2.2	<0.034	<0.15	<0.13
2-Heptanone	<0.070	2.3	<0.018	0.1	0.073
Nonane	<0.079	3.7	<0.020	<0.091	<0.079
Styrene (Ethenylbenzene)	<0.064	1.6	<0.017	<0.074	<0.064
Heptanal	<0.070	10	<0.018	0.12	0.074
o-Xylene	<0.065	1.5	<0.017	<0.076	<0.065
Cyclohexanone	<0.060	0.75	<0.016	<0.070	<0.060
1,1,2,2-Tetrachloroethane	<0.10	<0.14	<0.027	<0.12	<0.10
Octamethylcyclotetrasiloxane (OMCTS)	<0.30	<0.42	<0.079	1	0.4
1,3,5-Trimethylbenzene	<0.074	0.31	<0.019	<0.086	<0.074
1,2,4-Trimethylbenzene	<0.074	0.18	<0.019	<0.086	<0.074
1,3-Dichlorobenzene	<0.090	<0.13	<0.023	<0.10	<0.090
1,4-Dichlorobenzene	<0.090	<0.13	<0.023	<0.10	<0.090
1,2-Dichlorobenzene	<0.090	<0.13	<0.023	<0.10	<0.090
Decamethylcyclopentasiloxane (DMCPS)	<0.38	<0.53	<0.099	<0.44	<0.38
1,2,4-Trichlorobenzene	<0.19	<0.26	<0.048	<0.22	<0.19
Hexachlorobutadiene	<0.16	<0.22	<0.042	<0.19	<0.16

Target Compounds (TO-15)*	Lab 3 T3	Lab 3 R
1,1,1,2-Tetrafluoroethane	<0.10	<0.24
Perfluoro(2-methylpentane)	<0.21	<0.48
Propene	5.4	76
Propane	0.89	83
Carbonyl sulfide (Carbon oxide sulfide)	0.81	2.1
Freon 12 (Dichlorodifluoromethane)	<0.074	<0.17
Chloromethane	0.58	12
Freon 114 (1,2-Dichloro-1,1,2,2-tetrafluoro-ethane)	<0.10	<0.24
Isobutane	<0.036	2.1
Vinyl chloride	0.2	0.51
Methanol	<0.033	45
Acetaldehyde	0.37	628
2-Methyl-1-propene	0.86	90
Butane	0.44	38
1,3-Butadiene	<0.033	1.7
Bromomethane	<0.058	<0.13
Chloroethane	<0.040	12
Ethanol	<0.028	15
Freon 11 (Trichlorofluoromethane)	<0.084	<0.19
Propenal (Acrolein)	<0.034	126
Acetonitrile	<0.025	0.95
Acetone	0.22	109
Propanal (Propionaldehyde)	0.062	28
Furan	<0.042	61
Pentane	0.06	60
2-Propanol (Isopropanol)	<0.061	<0.14
Isoprene (2-Methyl-1,3-butadiene)	<0.042	0.25
1,1-Dichloroethene	<0.059	<0.14
Dimethyl sulfide	<0.038	0.86
Acrylonitrile	<0.033	8
Freon 113 (1,1,2-Trichloro-1,2,2-trifluoro-ethane)	<0.11	<0.26
2-Methyl-2-propanol	<0.045	0.17
Methyl acetate	<0.045	0.84
3-Chloropropene (Allyl chloride)	<0.047	0.23
Methylene chloride (Dichloromethane)	<0.052	<0.12
Carbon disulfide	0.6	16
1-Propanol	<0.037	1.2
Trimethylsilanol	<0.055	<0.13
1,1-Dichloroethane	<0.061	<0.14
Butanal (Butyraldehyde)	<0.044	103
2-Butanone (Methyl ethyl ketone)	0.055	36

Target Compounds (TO-15)*	Lab 3 T3	Lab 3 R
Hexane	<0.053	13
2-Methylfuran	<0.050	16
cis-1,2-Dichloroethene	<0.059	<0.14
Ethyl acetate	<0.054	0.48
Chloroform	<0.073	<0.17
1,1,1-Trichloroethane	<0.082	<0.19
2-Butenal	<0.043	3.8
1,2-Dichloroethane	<0.061	0.41
Benzene	<0.048	95
Carbon tetrachloride	<0.094	<0.22
1-Butanol	<0.045	1.4
2-Methylhexane	<0.061	0.17
2,3-Dimethylpentane	<0.061	0.26
3-Methylhexane	<0.061	0.18
2-Pentanone	<0.053	32
Pentanal	<0.053	39
n-Heptane	<0.061	14
Trichloroethene	<0.081	<0.19
1,2-Dichloropropane	<0.069	<0.16
2,5-Dimethylfuran	<0.059	2.2
1,4-Dioxane	<0.054	0.36
4-Methyl-2-pentanone (MIBK)	<0.061	5
cis-1,3-Dichloropropene	<0.068	<0.16
2-Pentenal	<0.052	4.8
trans-1,3-Dichloropropene	<0.068	<0.16
Toluene	<0.057	27
1,1,2-Trichloroethane	<0.082	<0.19
Mesityl oxide (4-Methyl-3-penten-2-one)	<0.060	2.7
Octane	<0.070	6.6
Hexanal	<0.061	18
Butyl acetate	<0.071	0.23
Tetrachloroethene (Perchloroethene)	<0.10	<0.23
1,2-Dibromoethane (EDB)	<0.12	<0.27
Chlorobenzene	<0.069	0.21
Ethylbenzene	<0.065	3.2
m & p-Xylene	<0.13	2.5
2-Heptanone	<0.070	2.4
Nonane	<0.079	3.8
Styrene (Ethenylbenzene)	<0.064	1.1
Heptanal	<0.070	7.1
o-Xylene	<0.065	1.3
Cyclohexanone	<0.060	0.74

Target Compounds (TO-15)*	Lab 3 T3	Lab 3 R
1,1,2,2-Tetrachloroethane	<0.10	<0.24
Octamethylcyclotetrasiloxane (OMCTS)	<0.30	<0.70
1,3,5-Trimethylbenzene	<0.074	1.7
1,2,4-Trimethylbenzene	<0.074	0.22
1,3-Dichlorobenzene	<0.090	<0.21
1,4-Dichlorobenzene	<0.090	<0.21
1,2-Dichlorobenzene	<0.090	<0.21
Decamethylcyclopentasiloxane (DMCPS)	<0.38	<0.87
1,2,4-Trichlorobenzene	<0.19	<0.43
Hexachlorobutadiene	<0.16	<0.37

Formulation of OSCAR Waste Simulant (OWS), the waste simulant used for this study.

Waste Material	% of OWS (wt%)
Clothing (cotton t-shirt)	17.9%
Food Packaging (FP)	13.4%
FP Overwrap	13.4%
Cotton towel	9.5%
Tech Wipes	3.6%
Toilet Paper	3.6%
Nitrile Gloves	1.6%
Fecal Simulant	13.4%
Wet Wipes	10.8%
Food Simulant	10.6%
Toothpaste	1.2%
Shampoo	1.2%