The Interaction of Spacecraft Cabin Atmospheric Quality and Water Processing System Performance

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ABSTRACT

Although designed to remove organic contaminants from a variety of waste water streams, the planned U.S.- and present Russian-provided water processing systems onboard the *International Space Station* (*ISS*) have capacity limits for some of the more common volatile cleaning solvents used for housekeeping purposes. Using large quantities of volatile cleaning solvents during the ground processing and in-flight operational phases of a crewed spacecraft such the *ISS* can lead to significant challenges to the water processing systems. To understand the challenges facing the management of water processing capacity, the relationship between cabin atmospheric quality and humidity condensate loading is presented. This relationship is developed as a tool to determine the cabin atmospheric loading that may compromise water processing system performance. A comparison of cabin atmospheric loading with volatile cleaning solvents from *ISS*, *Mir*, and Shuttle are presented to predict acceptable limits to maintain optimal water processing system performance.

BACKGROUND

The planned U.S.- and present Russian-provided water processing systems onboard the *International Space Station* (*ISS*) have a limited capacity for removing polar volatile organic compounds (VOCs) which can carry over from the cabin atmosphere into humidity condensate. Though the water processing systems are designed to remove polar VOCs from wastewater streams, using large quantities of these compounds in the cabin during flight operations may load the ISS humidity condensate to levels beyond the water processors' capacity. Polar VOCs of primary concern include methanol; ethanol; 2-propanol (isopropanol); n-propanol; n-butanol; 2-propanone (acetone); 1,2-ethanediol (ethylene glycol); 1,2-propanediol (propylene glycol); and 1,2,3-propanetriol (glycerol). These compounds can originate from equipment offgassing, crew metabolism, and crew activities. Careful attention to materials selection and control as well as controlled solvent use during manufacturing and pre-flight ground processing can minimize the polar VOC load from offgassing. This is the goal of the materials selection and control process combined with a good ground processing contamination control plan. The crew metabolic load can fluctuate according to crew size, activity level, and from person-to-person. These fluctuations tend to be moderate; therefore, the metabolic polar VOC load is considered fairly static on average. In-flight polar VOC generation from crew activities can fluctuate widely unless strict controls on their use are in place.

Controls imposed during Shuttle and Spacelab missions typically focus upon proper containment to prevent excessively large releases into the cabin. This approach minimizes the risk that a release could result in exceeding individual compound Spacecraft Maximum Allowable Concentrations (SMACs). While these controls address safety and acute health effects, the policy using volatile solvents for cleaning and personal hygiene purposes onboard the Shuttle and Spacelab has been liberal. This has not presented a significant problem to these programs because the humidity condensate is not recycled for the crew's use. This situation changes significantly when the condensate is recycled.

NASA's recent participation in the Shuttle-*Mir* Program was the U.S. space program's first experience with the inherent sensitivities of onboard water processing systems to in-flight polar VOC use by the crew. Typically, products containing polar VOCs such as low molecular weight alcohols were not permitted onboard *Mir* because they load humidity condensate significantly and are difficult to remove from water once in it. Essentially a duplicate of *Mir*'s water processor is onboard the *ISS* Service Module (SM), *Zvezda*. This means that the sensitivities to alcohol use that were characteristic of *Mir*

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apply to the *ISS* after station assembly flight 2R. Therefore, the issue of polar VOC use by the crew is an immediate issue to be addressed.

Onboard trace contaminant control (TCC) systems located in *Zvezda* and the U.S. Laboratory, *Destiny*, are designed to handle the basic cabin air loads produced by offgassing and crew metabolism. These systems include design margin that can handle the added load produced by crew activities such as housekeeping, maintenance, food preparation and consumption, personal hygiene, and experimental facility operations. The baseline TCC systems, however, are not the only processes which removed VOCs from the cabin atmosphere. System-level testing has demonstrated that absorption in humidity condensate is a significant removal route.[1] Because the *ISS* water processing equipment must remove the polar VOCs from this waste water source as well as other waste sources to provide the crew with a potable water supply, attention must be placed upon further limiting their in-flight use by the crew. The U.S. Segment Water Processor's (WP) capability to handle a well-defined polar VOC design load has been demonstrated. However, their use by the crew represents an additional load for which the effects on the WP's ability to meet the potable water quality requirements must be evaluated. The following analysis addresses the generation of several polar VOCs produced by typical crew activities and the effect of varying rates of production on their concentration in humidity condensate.

RELATION OF CABIN ATMOSPHERIC QUALITY AND CONDENSATE LOADING

A mass balance on a typical condensing heat exchanger, assuming co-current condensate and process air flow, provides a general equation relating bulk liquid (condensate) and gas (atmospheric) phase mole fraction.[4] Equation 1 shows the basic form solved for liquid phase mole fraction. In equation 1, x is the VOC liquid phase mole fraction, y is the VOC gas phase mole fraction, C is the condensate flow rate in the heat exchanger core in moles/hour, A is the process air flow rate through the heat exchanger core in moles/hour, H is the Henry's Law constant in atm/mole fraction, and P is total pressure in atmospheres. Recent testing has shown that for highly polar compounds, an adjustment, α, to the Henry's Law constant is necessary to account for the 10 °C heat exchanger operating temperature and liquid phase interactions.[5]

$$x = \frac{y}{C/A + \alpha H/P} \qquad (1)$$

The liquid phase mole fraction, x, can be expressed by equation 2 in which n_i is the number of moles of the dilute VOC and n_w is the number of moles of water. In equation

2, the total moles of water is 55.5 for a 1-L condensate basis. The contribution from the dilute VOC is considered negligible and does not significantly change the total moles of water. The number of moles is defined by the liquid phase concentration in mg/L, C_L, divided by molecular weight, M, in g/mole and a unit conversion of 10^3 mg/g as shown by equation 3. Substituting equation 3 and total moles of water into the definition of mole fraction yields equation 4.

$$x = \frac{n_i}{n_w + n_i} \qquad (2)$$

$$n_i = \frac{C_L}{10^3 M} \qquad (3)$$

$$x = \frac{C_L / 10^3 M}{55.5 + C_L / 10^3 M} \qquad (4)$$

Similarly, assuming that the ideal gas law applies to dilute contaminants, the gas phase mole fraction, y, can be defined by equation 5. Unit conversions of 10^3 mg/g and 10^6 cm³/m³ are applied in the denominator. The ideal gas constant, R, is 82.06 cm³-atm/mole-K and total pressure, P, is 1 atmosphere. The temperature, T, is set at the condenser's operating temperature of 283 K. The atmospheric concentration, C_A, is in units of mg/m³ while the molecular weight, M, is in units of g/mole.

$$y = \frac{C_A RT}{10^9 MP} \qquad (5)$$

Combining equations 1, 4, and 5 in addition to applying the appropriate constants and solving for C_A yields equation 6. Using equation 6 along with the physical constants in Table 1, an estimate of the cabin

$$C_A = \frac{43,060.8 M C_L}{55,500 M + C_L}(0.000362 + \alpha H) \qquad (6)$$

air concentration that can produce a specific condensate loading can be made. Water processor design condensate loading for the four compounds of interest are listed by Table 2 along with the associated cabin atmospheric concentration necessary to produce them. The WP condensate design load was developed to reflect the anticipated composition of the *ISS* condensate. The data are based upon analyses of condensate samples collected from the Shuttle, Spacelab, and developmental testing at the NASA's Marshall Space Flight Center (NASA MSFC).

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Table 1. Physical and Experimental Constants for Selected Compounds

COMPOUND	MOLECULAR WEIGHT (g/mole)	HENRY'S CONSTANT (atm)	SHAPE FACTOR (α)
Methanol	32.04	0.39	0.38
Ethanol	46.07	0.45	0.40
Isopropanol	60.09	0.62	0.40
n-propanol	60.09	0.51	0.40
n-butanol	74.12	1.36	0.40
Acetone	58.08	2.38	0.54
Ethylene glycol	62.07	0.0001	0.40
Propylene glycol	76.10	0.0833	0.40
Glycerol	92.10	0.0007	0.40

Table 2. Condensate and Atmospheric Loading

COMPOUND	CONDENSATE DESIGN LOAD (mg/L)	ATMOSPHERIC CONCENTRATION (mg/m^3)	SMAC (mg/m^3)
Methanol	3.1102	0.35	9
Ethanol	6.1156	0.86	2,000
Isopropanol	38.3327	7.4	150
n-propanol	0.1986	0.031	98
n-butanol	0.9368	0.4	80
Acetone	3.9642	4	50
Ethylene glycol	8.6974	0.0027	13
Propylene glycol	35.0483	0.92	NA
Glycerol	2.8320	0.0014	NA

Table 2 shows that the individual contaminant atmospheric concentrations that can result in condensate loading at the water processor's design level are well below their respective SMACs. The materials selection and control process passively limits trace contaminant generation via offgassing while the onboard trace contaminant control systems remove the crew metabolic, residual offgassing, and other miscellaneous loads from crew activities to low levels. The load of the primary generation sources—crew metabolism and equipment offgassing—versus the trace contaminant removal capability must be assessed to determine the margin that exists to accommodate generation from the various crew activities.

It should be noted that the atmospheric concentrations listed in Table 2 for ethylene glycol and glycerol fall below the typical analytical method detection limit in air of 0.05 mg/m^3. Therefore, it is possible for these compounds to be in the cabin atmosphere at concentrations that are deleterious to the WP's performance but not detected in archival grab samples.

CONTAMINANT GENERATION SOURCES

Trace atmospheric contamination in a spacecraft cabin can originate from many sources.[6] Chief among these are materials offgassing and human metabolism. Other major sources are from crew activities such as housekeeping, food preparation and consumption, personal hygiene, and payload operations. Table 3 lists predicted hourly offgassing rates derived from element offgassing tests conducted through STS-100/6A and those predicted for the ISS at assembly complete. The assembly complete case applies offgassing rates derived from Node 1 flight element offgassing test data to 75,000 kg of internal hardware and metabolic loading reported by reference 7 applied to 6 people. Glycerol's rate is derived from its evaporation rate from a shallow pool having a 1-m^2 surface area.[8] The total rates for both cases were evaluated to determine the predicted cabin concentration in the *ISS* at its present assembly stage and at assembly complete. Predicted concentrations are compared with the atmospheric concentrations from Table 2 that correspond to the WP's condensate load limits. To evaluate additional polar VOC use by the crew, the base rates were increased by 1,000 mg/day.

Table 3. Base Contaminant Generation Rates

COMPOUND	CONCLUSION OF STS-100/6A			ASSEMBLY COMPLETE		
	OFFGASSING RATE (mg/h)	METABOLIC RATE (mg/h)	TOTAL RATE (mg/h)	OFFGASSING RATE (mg/h)	METABOLIC RATE (mg/h)	TOTAL RATE (mg/h)
Methanol	1.6	0.11	1.71	0.73	0.22	0.95
Ethanol	10.9	0.55	11.4	16.4	1.1	17.5
Isopropanol	3.37	0.21	3.58	15.4	0.42	15.8
n-propanol	0.36	0.07	0.43	0.75	0.14	0.89
n-butanol	1.55	0.065	1.62	14.7	0.13	14.8
Acetone	3.15	2.35	5.5	4.0	4.7	8.7
Ethylene glycol	0	0	0	0.0188	0	0.0188
Propylene glycol	0	0	0	0.0008	0	0.0008
Glycerol	0	0	0	0.00146	0	0.00146

TRACE CONTAMINANT REMOVAL DEVICES

The *ISS* cabin free volume is estimated to be approximately 300 m³ as of STS-100/6A and will increase to approximately 644 m³ once completed. Presently, the *ISS* trace contaminant removal capability consists of 1 Trace Contaminant Control Subassembly (TCCS) unit in *Destiny* and 1 BMP unit in *Zvezda*. Normally, two condensing heat exchangers are operating to control cabin temperature and relative humidty.

At assembly complete, the *ISS* will contain 2 TCCS units, 1 BMP, and up to 7 condensing heat exchangers. For the purpose of the assembly complete case of this analysis, it has been assumed that 4 condensing heat exchangers are the primary contributors to the latent heat removal and 1 TCCS unit will be operating at any given time in parallel with the BMP. These units will remove contamination generated at the rates listed by Table 3 plus that generated by crew activities.

The TCCS removes trace contaminants via physical adsorption by activated charcoal and high temperature catalytic oxidation. Process air flow through the charcoal bed is 15.29 m³/h and through the oxidizer is 4.59 m³/h. The BMP also removes contaminants via physical adsorption but instead of using a high temperature catalytic oxidizer, it uses an ambient temperature catalyst to oxidize carbon monoxide. The flow through the BMP is 27 m³/h.

It has been assumed that the daily latent load of 1.6 L/day-person is divided between 4 condensing heat exchangers at assembly complete and 2 heat exchangers for the STS-100/6A case. Based on flight data, approximately 0.02 kg condensate/h is being removed by the heat exchanger in *Destiny* while 0.27 kg condensate/h is being removed by *Zvezda's* heat exchanger. A similar loading is used for assembly complete with 2 exchangers removing condensate at the

higher rate to account for greater time spent by the crew in some parts of the station. Process air flow is 680 m³/h through the U.S. Segment central ventilation system and 600 m³/h through the Russian Segment ventilation system. Up to 90% of the total air flow bypasses the heat exchanger core in the U.S. Segment unit in the configuration to maximize condensate collection in the Russian Segment. Similarly, approximately 76% of the total air flow in the Russian Segment ventilation system bypasses the heat exchanger. Therefore, the actual process air flow through the U.S. Segment and Russian Segment heat exchanger cores is approximately 68 m³/h and 144 m³/h, respectively.

CALCULATION APPROACH

Information on the *ISS* configuration, TCCS, BMP, and condensing heat exchangers along with physical properties properties of the contaminants of interest are used as input to a cabin mass balance model, the Trace Contaminant Control Simulation Computer Program (TCCS CP).[9] The TCCS CP solves the cabin mass balance, summarized by equation 7, using a backwards differencing technique. In equation 7, C_i is the individual contaminant concentration, g_i is the generation rate, η is the removal device efficiency, v is the device volumetric flow rate, t is time, and V is the cabin volume.

$$C_i = C_{i,o} e^{-\eta v t / V} + (g_i / \eta v)(1 - e^{-\eta v t / V}) \qquad (7)$$

Two cases are investigated for the STS-100/6A and assembly complete configurations. The first case uses the base contaminant generation rates listed by Table 3 while the second case uses rates that are increased by 1 gram/day across the board. The difference between the concentrations are determined for the 2 configurations then divided by the generation rate difference. This number is the slope of the curve relating contaminant generation rate to cabin concentration. For simplicity, this curve is assumed to be linear with a y-intercept at zero.

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Using the threshold cabin concentrations that correspond to the WP's design limit from Table 2, the corresponding threshold generation rate is determined by either interpolation or extrapolation. The base rates are then subtracted to arrive at the additional generation above the base that is allowable for housekeeping and other crew activities. In addition, the same cases were run for the U.S. Segment only to bound the range of allowable daily VOC use.

RESULTS

Results from the system-level analysis are summarized in Tables 4 and 5. The calculated delta rate is the difference between the base rate and the rate that results in individual cabin concentrations equal to those listed by Table 2. Table 4 shows that the *ISS's* full atmospheric scrubbing capability can accommodate approximately 13 grams/day of additional polar VOC generation. This generation rate corresponds to a total polar VOC concentration of approximately 13.9 mg/m³ as obtained by summing the atmospheric concentrations in

Table 2. Individually, no single contaminant has exceeded its maximum allowable rate.

The situation changes when considering the scrubbing capability of only the U.S. Segment. At the completion of Phase II, the U.S. Segment can accommodate approximately 4.7 grams/day above the base generation rates. This decreases, however, to as low as 3 grams/day above the base generation rates at assembly complete. The decrease occurs because the U.S. Segment's scrubbing capacity remains static while the projected base alcohol loading from equipment offgassing and human metabolism increase due to additional equipment and a larger crew size. Projected increases in n-butanol and 2-propanol offgassing rates are the primary drivers. As well, during all *ISS* assembly phases, the low molecular weight alcohols will rapidly saturate the expendable charcoal bed leaving the catalytic oxidizer as the primary removal device in the TCCS. The oxidizer flow, at 4.6 m³/h, is only one-third of the flow through the charcoal bed and the result is a lower removal rate. The 13.9 mg/m³ total polar VOC concentration also applies to this case.

Table 4. Station-level Polar VOC Usage Rates

COMPOUND	CONCLUSION OF STS-100/6A			ASSEMBLY COMPLETE		
	CONCENTRATION DELTA (mg/m³)	MAXIMUM RATE (mg/h)	DELTA RATE (mg/day)	CONCENTRATION DELTA (mg/m³)	MAXIMUM RATE (mg/h)	DELTA RATE (mg/day)
Methanol	4.91	2.93	29.3	4.00	3.6	63.5
Ethanol	1.34	26.57	364	1.26	28.32	259.9
Isopropanol	0.96	320.2	7598	0.93	329	7517
n-propanol	0.98	1.34	21.9	0.98	1.34	10.8
n-butanol	0.98	16.74	363	0.98	16.79	47.7
Acetone	0.98	168.2	3904	0.98	168.7	3840
Ethylene glycol	0.17	0.65	15.7	0.12	0.98	23.1
Propylene glycol	0.92	41.35	992.4	0.87	44.06	1057
Glycerol	0.20	0.3	7.1	0.13	0.44	10.6
	TOTAL VOC RATE		13295.4	TOTAL VOC RATE		12829.6

Table 5. U.S. Segment-level Polar VOC Usage Rates

COMPOUND	CONCLUSION OF STS-100/6A			ASSEMBLY COMPLETE		
	CONCENTRATION DELTA (mg/m³)	MAXIMUM RATE (mg/h)	DELTA RATE (mg/day)	CONCENTRATION DELTA (mg/m³)	MAXIMUM RATE (mg/h)	DELTA RATE (mg/day)
Methanol	8.48	1.7	-0.28	5.60	2.57	38.9
Ethanol	7.04	5.1	-152.1	5.99	5.95	-277.3
Isopropanol	2.08	148.3	3474	2.45	125.5	2632
n-propanol	2.09	0.63	4.8	2.58	0.51	-9.2
n-butanol	2.09	7.9	150.3	2.67	6.17	-207.1
Acetone	4.54	36.3	739.4	6.34	25.96	414.3
Ethylene glycol	0.33	0.35	8.3	0.10	1.13	26.6
Propylene glycol	2.04	18.7	449.6	2.05	18.59	446.1
Glycerol	0.43	0.14	3.3	0.12	0.5	11.9
	TOTAL VOC RATE		4677.3	TOTAL VOC RATE		3076.2

COMPARISON TO FLIGHT EXPERIENCE

ATMOSPHERIC LOADING – To understand how well the base predictions correlate to actual *ISS* operations, the past and present on-orbit experience regarding atmospheric trace contaminant loading must be examined. Concentration data collected during *ISS* missions 5A and 5A.1 that reflect the station's total scrubbing capability are summarized by Table 6.[10, 11] These data are consistent with the base offgassing and human metabolic loading used for the analysis because few logistics flights had yet occurred. In addition, all of the available trace contaminant control equipment was operating as of mission 5A giving a good representation of joint U.S. and Russian equipment operation. As can be seen, the predicted concentrations are lower by an average factor of 2.7 relative to the measured in-flight atmospheric quality. This means that actual generation is higher than the available equipment offgassing data indicate.

Average observed concentrations for the Shuttle from 100 grab samples, for Spacelab from 43 grab samples, and for *Mir* from 87 grab samples are summarized by Table 7.[12-20] Comparison of the average concentrations from Table 7 to analysis results in Table 6 indicate that the atmospheric concentrations onboard the *ISS* are being controlled to similar levels or better than previous space programs.

Further comparison of the reported concentrations from *Mir* to the average concentrations observed to date onboard the *ISS* indicate that some net increase in most steady state atmospheric concentrations should be expected. Methanol is an exception as its early offgassing rate has been quite high. Air quality data from the *ISS* do show that methanol's offgassing decayed significantly between the time that the ground-based offgassing test was conducted on *Unity* and the first early ingress during STS-88/2A approximately 2 months later.[21] It is expected that methanol's offgassing rate will continue to decay and cabin concentrations should not rise appreciably through the remainder of *ISS* assembly.

This typical offgassing rate behavior will be repeated with every new station element deployed so that atmospheric concentration peaks are expected. Once station operations become more routine and its habitable configuration more stable, it is anticipated that an average atmospheric trace contaminant load representative of that observed during Shuttle, Spacelab and *Mir* missions will prevail. The concentration range observed in flight from these 3 programs indicate that the results of the analysis of polar VOC control capability can be used to reach a sound conclusion concerning constraints on their use during crew activities.

Table 6. Predicted versus Observed Concentrations at STS-106/6A

COMPOUND	SMAC (mg/m^3)	PREDICTED (mg/m^3)	*ISS* (mg/m^3)
Methanol	9	0.058	0.09
Ethanol	2,000	0.28	1.43
Isopropanol	150	0.084	0.14
n-propanol	98	0.01	0.025
n-butanol	80	0.038	0.15
Acetone	50	0.13	0.16

Table 7. Average Shuttle, Spacelab, and *Mir* Atmospheric Concentrations

COMPOUND	SMAC (mg/m^3)		SHUTTLE (mg/m^3)	SPACELAB (mg/m^3)	*MIR* (mg/m^3)
	NASA	RUSSIAN			
Methanol	9	0.2	0.04	0.05	0.21
Ethanol	2,000	10	2.8	2.0	1.6
Isopropanol	150	1.5	2.0	4.5	0.51
n-propanol	98	0.6	0.014	0.031	0.024
n-butanol	80	0.8	0.031	0.077	0.26
Acetone	50	2	0.83	0.46	0.48

CONDENSATE LOADING – To complete the comparison between predicted atmospheric loading and humidity condensate loading, it is also necessary to consider results from humidity condensate analyses. Table 8 shows the condensate loading for a sample returned on STS-104/7A and two samples collected during Increment 3 and returned on STS-108/UF-1. The first sample was collected on 19 July 2001, the second on 6 September, and the third on 24 November. All three samples were collected in the U.S. Segment. Equation 6 was used to calculate the atmospheric loading that corresponds to the measured humidity condensate loading. Reported atmospheric concentrations from samples collected as close as possible to the time the condensate samples are used as a comparison to that calculated from the humidity condensate loading. This approach allows for a second basis for evaluating polar VOC use to be considered.

The sample collected on 6 September shows loading that is comparable to that collected on 19 July. Exceptions are higher acetone and n-propanol loading as well as markedly lower ethylene glycol and propylene glycol loading. The sample collected on 24 November shows loading similar to the one collected on 6 September except that ethanol loading is nearly 50% higher.

Comparison shows that the measured humidity loading indicates a higher atmospheric loading than measurements indicate for all three data sets. Predicted atmospheric concentrations for methanol, ethanol, n-propanol, and acetone corresponding to the humidity condensate loading reported in the sample collected on 19 July are greater than those reported from flight grab samples by an average factor of 3.4. Isopropanol's predicted atmospheric concentration is 6 times higher

than measured while the predicted concentration for n-butanol is 10.3 times higher than measured. Weighted with respect to the total condensate loading, the predicted atmospheric loading is approximately 4 times higher than was measured in grab samples for the sample collected on 19 July. Similarly, the predicted atmospheric concentrations corresponding to the condensate loading reported in the samples collected on 6 September and 24 November are approximately 3 and 1.6 times higher, respectively, than measured in the grab samples.

There may be many reasons why the condensate loading indicates a higher cabin atmosphere loading that what has been measured. Relative analytical errors may contribute as well as liquid phase interactions such as hydrogen bonding that possible may become enhanced in microgravity conditions. Another possible explanation is that the grab sampling technique provides only an indication of atmospheric loading at a single point in time. Sustained peaks in loading can be missed by the technique whereas the condensate loading indicates a time-integrated sample that includes the effects of peaks in atmospheric loading. To achieve better comparison, it is necessary to coordinate condensate and atmospheric sampling to be done within the same hour. Although many hypotheses may be presented about the cause of the condensate and atmospheric loading differences, the available data do not allow for its root cause to be determined.

Overall, the difference must be considered as an indicator of uncertainty when setting polar VOC use limits. This is accomplished by conservatively adjusting the concentration limits associated with total polar VOCs downward by a factor of 3. The same adjustment also applies to allowable daily generation rates reported by Tables 4 and 5.

Table 8. Atmospheric Loading Indicated by the Measured Condensate Load

COMPOUND	STS-104/7A			INCREMENT 3a			INCREMENT 3b		
	C_L mg/L	C_A (mg/m^3)		C_L mg/L	C_A (mg/m^3)		C_L mg/L	C_A (mg/m^3)	
		Predicted	Measured		Predicted	Measured		Predicted	Measured
Methanol	6.87	0.76	0.22	6.32	0.70	0.54	6.9	0.77	0.64
Ethanol	50.4	7	2	47.7	6.67	2.28	71.3	9.98	6.2
Isopropanol	2.55	0.49	0.082	2.93	0.56	0.22	2.06	0.40	0.16
n-propanol	0.59	0.09	0.025	0.79	0.12	0.05	0.66	0.10	0.06
n-butanol	2.88	1.22	0.12	2.4	1.01	0.14	1.43	0.60	0.13
Acetone	0.39	0.39	0.14	0.52	0.52	0.26	0.35	0.35	0.22
Ethylene glycol	11	0.0034	0	6.5	0.0020	0	7.08	0.0022	0
Propylene glycol	113	2.95	0	52	1.36	0	58.9	1.54	0
Glycerol	0	0	0	0	0	0	0	0	0

* Reported from samples returned on STS-104/7A

CONTAMINATION DYNAMICS AND DISTRIBUTION ONBOARD *ISS*

Figure 1 shows the total VOC loading in the *ISS* cabin throughout the station's early assembly stages beginning with STS-88/2A in December 1998, continuing through STS-108/UF-1 in December 2001. As can be seen, higher concentrations were observed at the beginning of each ingress period.[22] [-27] After the station atmosphere dilutes with the Orbiter volume and continues to be scrubbed, lower concentrations comparable to those summarized by Table 6 are achieved. For example, at the conclusion of 2A.1 ingress operations, average cabin concentrations were 0.36 mg/m³, 2.35 mg/m³, 0.62 mg/m³, and 0.22 mg/m³ for methanol, ethanol, isopropanol, and acetone, respectively. Propanol was not detected but the n-butanol concentration grew from trace levels to an average of 0.26 mg/m³. Ethylene glycol, propylene glycol and glycerol have not been reported above detection limits.

With respect to total polar VOC concentration transients, three in-flight cases are noteworthy. The first is 2A.2a where the maximum isopropanol concentration reached 13 mg/m³. This concentration was measured from a sample collected at the end of the docked phase. Concentrations in the Orbiter approached 10 mg/m³ during the same time. This increase was indicative of in-flight isopropanol use by the crew. The second case, 2A.2b, saw ethanol as high as 25 mg/m³ during ingress of unscrubbed volumes in the PMA-1, *Zvezda*, and the Progress. The concentration across the *ISS* was reduced to 2.7 mg/m³ by the end of the docked phase. The third case occurred just before STS-105 was launched. It involved a methanol concentration of approximately 70 mg/m³ in a sampled collected in the *Zarya*. Samples were collected later and returned on a Soyuz vehicle showed the methanol had been reduced to nearly 2 mg/m³. The methanol's source was not determined.

The high ethanol concentrations during the first ingress operations during 2A.2b demonstrate the contamination potential of new modules and equipment. For this reason, VOC use during ground processing should be restricted close to final element closeout. Employing such a restriction is attributed to reducing the total VOC concentration in the MPLM at first ingress by half. The first flight of an MPLM, STS-102/5A.1, saw total VOCs at nearly 10 mg/m³ at first ingress. Subsequent MPLM flights, STS-100/6A, STS-105/7A.1, and STS-108/UF-1 reported total VOCs at approximately 5 to 6 mg/m³ at first ingress.

Even with precautions taken, concentration peaks are expected as new modules and equipment are added to the vehicle. As the hardware ages, average concentrations will decrease. Therefore, it is expected that cabin concentrations will decrease to magnitudes similar to those experienced on average during Shuttle, Spacelab, and *Mir* missions as the Russian Segment BMP onboard *Zvezda* and U.S. Segment TCCS onboard *Destiny* continue to operate.

The elevated methanol concentration in *Zarya* demonstrates that local transients are possible. Even so, the entire *ISS* cabin remains nearly well mixed with some noted exceptions. Figure 2 shows the total VOC distribution by module beginning with *Zvezda's* activation during mission 2R. As can be seen, the measured concentrations in *Zvezda* and *Destiny* follow each other closely indicating good ventilation exchange between them. An increasing trend is evident with significant peaks in *Zvezda* indicating local polar VOC use. As well, there are instances where the loading in *Zarya* is noticeably higher. This can be attributed to the fact that there is forced ventilation flow from *Zvezda* forward to *Unity* and *Destiny* but only plenum flow through the hatches into *Zarya*. Additionally, *Zvezda* and *Destiny* have local contamination and humidity control systems that remove the contaminants while *Zarya* has no active contamination control system normally operating. As a result, it is not surprising that local concentrations in *Zarya* occur.
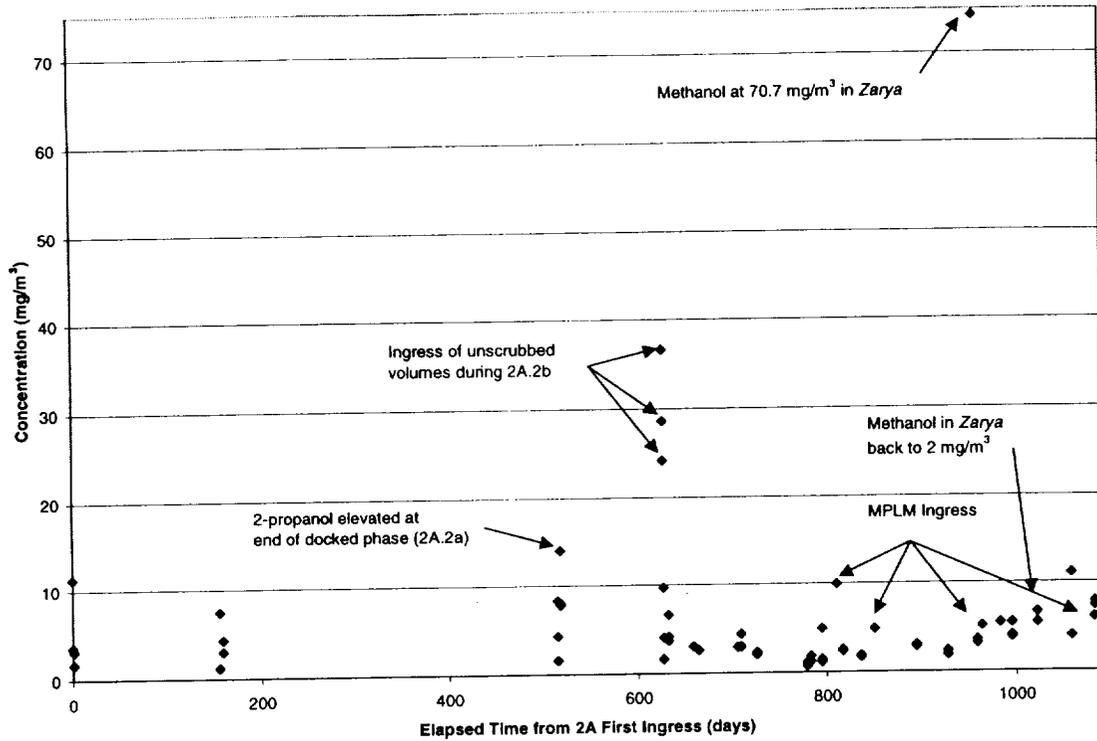
Figure 1. Total VOC Loading in the *ISS* Cabin
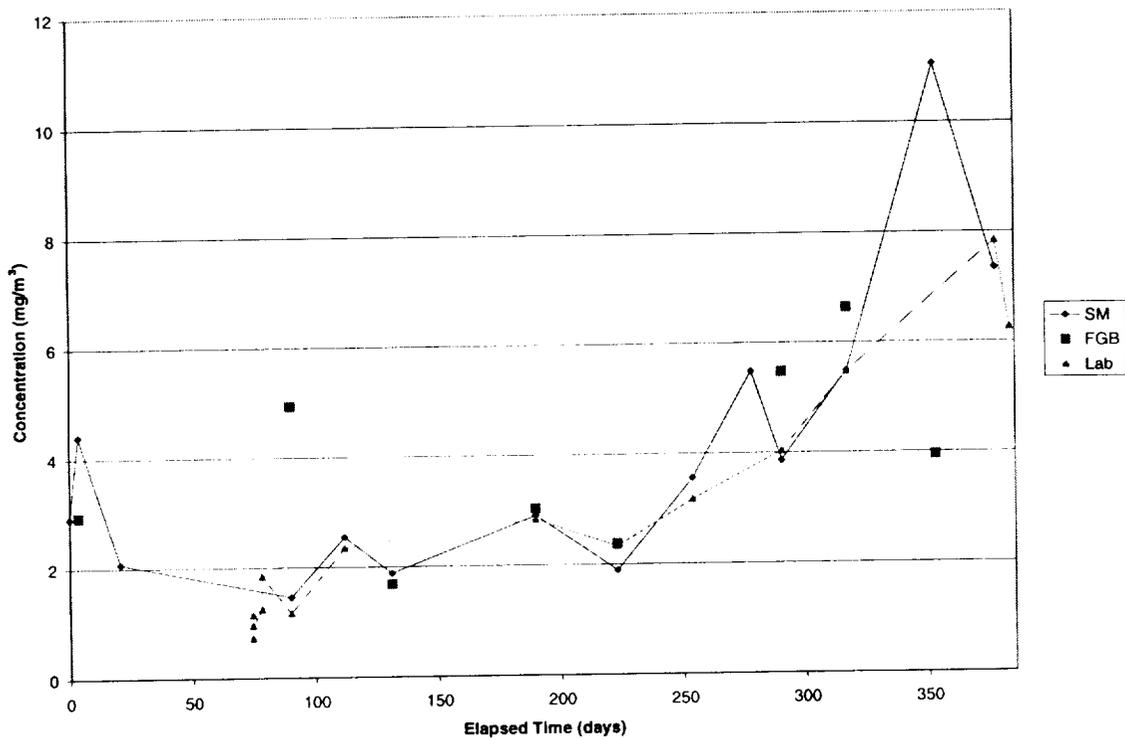
*Note that the peak of 70 mg/m³ at approximately day 250 is not shown. Elapsed time begins at *Zvezda* activation.

Figure 2. Spatial Distribution of VOCs Onboard the *ISS*

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CONDENSATE LOADING LIMITS

The limit for condensate loading specified for the Russian Segment water processor (Russian acronym CRV-K2M) is 100 mg total alcohols/L including 80 mg total ethanol and isopropanol/L. This compares to the total alcohol limit of 99.24 mg/L for the U.S. Segment water processor. The U.S. design specification has a more stringent limit for total ethanol and isopropanol of 44.45 mg/L. Compared to the U.S. WP's total polar VOC design specification of 13.9 mg/m^3, the CRV-K2M is capable of handling a slightly higher concentration – 15.1 mg/m^3. Based upon this comparison, it is reasonable to apply the conclusions and recommendations of the polar VOC usage assessment to the entire *ISS*. Typically, the total polar VOC loading has been maintained below 10 mg/m^3 with the exception of the noted cases. Considering the observed difference between humidity condensate and atmospheric loading, the total polar VOC loading concentration limit in the range between 4.6 mg/m^3 and 5 mg/m^3. The lower limit of this range, 4.6 mg/m^3, is therefore a reasonable limit. For simplicity, rounding the limit to 5 mg/m^3 is recommended.

CONCLUSIONS

When using equipment offgassing data and atmospheric quality as the primary basis to evaluate the polar VOC removal capacity and considering the evaluation of past and present flight atmospheric trace contaminant loading data, the total allowable polar VOC usage rate for the *ISS* is 13 grams/day with no more than 3 grams/day of this within the U.S. Segment. The atmospheric concentration for total low molecular weight alcohols and acetone should not exceed 14 mg/m^3 to protect the onboard water processing systems. The conditions onboard the *ISS* are presently well below this limit.

However, when using measured humidity condensate loading as the primary evaluation basis, the difference between measured condensate and atmospheric loading must be considered. Accounting for this difference, the total polar VOC usage rate for the entire *ISS* may be as low as 4 grams/day with no more than 1 gram/day of this generated within the U.S. Segment. The allowable cabin concentration decreases to 5 mg/m^3. The conditions onboard the *ISS* are presently exceeding this allowable concentration.

Clearly, these results demonstrate that cabin atmospheric quality must be considered when designing water recovery and processing systems. As well, conservative design practice must consider the condensate loading as the basis. By using techniques developed in this study, a robust water processing system design can be obtained.

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