Impacts of an Ammonia Leak on the Cabin Atmosphere of the International Space Station

Stephanie M. Duchesne¹
Wyle Integrated Sciences and Engineering, Houston, TX, 77058

and

Jeffrey J. Sweterlitsch, Ph.D.²
National Aeronautic and Space Administration (NASA) Johnson Space Center (JSC), Houston, TX, 77058

and

Chang H. Son, Ph.D.³
The Boeing Company, Houston, TX, 77059

and

Jay L. Perry⁴
National Aeronautic and Space Administration (NASA) Marshall Space Flight Center (MSFC), Huntsville, AL, 35811

Toxic chemical release into the cabin atmosphere is one of the three major emergency scenarios identified on the International Space Station (ISS). The release of anhydrous ammonia, the coolant used in the U.S. On-orbit Segment (USOS) External Active Thermal Control Subsystem (EATCS), into the ISS cabin atmosphere is one of the most serious toxic chemical release cases identified on board ISS. The USOS Thermal Control System (TCS) includes an Internal Thermal Control Subsystem (ITCS) water loop and an EATCS ammonia loop that transfer heat at the interface heat exchanger (IFHX). Failure modes exist that could cause a breach within the IFHX. This breach would result in high pressure ammonia from the EATCS flowing into the lower pressure ITCS water loop. As the pressure builds in the ITCS loop, it is likely that the gas trap, which has the lowest maximum design pressure within the ITCS, would burst and cause ammonia to enter the ISS atmosphere. It is crucial to first characterize the release of ammonia into the ISS atmosphere in order to develop methods to properly mitigate the environmental risk. This paper will document the methods used to characterize an ammonia leak into the ISS cabin atmosphere. A mathematical model of the leak was first developed in order to define the flow of ammonia into the ISS cabin atmosphere based on a series of IFHX rupture cases. Computational Fluid Dynamics (CFD) methods were then used to model the dispersion of the ammonia throughout the ISS cabin and determine localized effects and ventilation effects on the dispersion of ammonia. Lastly, the capabilities of the current on-orbit systems to remove ammonia were reviewed and scrubbing rates of the ISS systems were defined based on the ammonia release models. With this full characterization of the release of ammonia from the USOS TCS, an appropriate mitigation strategy that includes crew and system emergency response procedures, personal protection equipment use, and atmosphere monitoring and scrubbing hardware can be established.

¹ ISS Environmental Control and Life Support Systems Subsystem Manager, EC6 Crew and Thermal Systems Division, 1290 Hercules Avenue Suite 120, Houston, TX, 77058.
² Insert Job Title, Department Name, Address/Mail Stop, and AIAA Member Grade for second author.
³ Insert Job Title, Department Name, Address/Mail Stop, and AIAA Member Grade for fourth author (etc).
⁴ Insert Job Title, Department Name, Address/Mail Stop, and AIAA Member Grade for fourth author (etc).

American Institute of Aeronautics and Astronautics
Nomenclature

atm = Atmosphere
°C = Celsius
°F = Fahrenheit
g = Grams
in = Inch
kg = Kilograms
kPa = Kilopascal
mm = Millimeters
m³ = Cubic meters
ppm = Parts per million
psi = Pounds per square inch

I. Introduction

There are three classes of emergencies identified on the International Space Station (ISS): Fire, Depressurization and Toxic Release. In the case of a toxic release, a leak of Ammonia into the cabin atmosphere from the External Active Thermal Control System (EATCS) is considered the most catastrophic for both crew health and vehicle. Though this type of a leak is considered low probability, the consequence justifies steps to mitigate the hazard magnitude. To this end, it is necessary to understand the mechanism for ammonia entry into the cabin atmosphere, the dispersion rate of ammonia through the ISS cabin, and the capability to remove ammonia from the atmosphere once the leak is isolated. A detailed description of the ammonia chemistry, and ISS ammonia leakage scenarios are discussed in Ref 1.

II. Ammonia Release into the ISS Atmosphere: EATCS IFHX Rupture

The largest source of ammonia aboard ISS resides in the EATCS which provides heat rejection for the U.S. On-orbit Segment (USOS) and International Partner (IP) modules. Ammonia is not used on the Russian On-orbit Segment (ROS). The EATCS is a pumped single-phase ammonia system that collects heat from cold plates and heat exchangers and rejects it to space. The internal thermal control system (ITCS) uses pumped single-phase water to remove heat from USOS and IP systems and payloads and rejects heat to the EATCS via an interface heat exchanger (IFHX). The ITCS consists of a low temperature loop (LTL) and a moderate temperature loop (MTL). The lowest design pressure within the ITCS is the gas trap located in the pump package assembly. For this reason, it is theorized that the gas trap would be the point of entry of ammonia into the ISS cabin as the ITCS loop overpressurizes after the IFHX failure. There are six prime gas traps aboard the USOS: 2 in the US Lab, 2 in Node 2, and 2 in Node 3.

Hazard assessments identified three scenarios that could lead to a breach in the water/ammonia barrier of the IFHX that in turn would cause high pressure ammonia to pass from the EATCS into the ITCS and then into the cabin: 1) IFHX core freeze/thaw, 2) Structural Failure of the IFHX, or 3) Over-pressurization of the IFHX. The IFHX has a low probability of failing due to proper selection of materials, design, and testing as well as the inclusion of relief valves, bleed lines, software controls and procedures. The existing NASA probabilistic risk assessment (PRA) model shows that the likelihood of an ammonia leak due to IFHX core freezing is 1 in 1,406,074.² Assuming proper software control and procedures are followed, that number drops to 10⁻¹⁹.²
The IFHX failure scenario is broken down into 3 types of leaks: micro leak, moderate leak, and rupture. The micro leak is considered the result of micro cracks or corrosion of the IFHX and is detected through periodic sampling of the ITCS water loop. Remediation steps are taken as necessary upon detection. A moderate leak is detected through monitoring of the ITCS accumulator quantity. This type of leak could be detected through sampling of the ITCS, crew sense of smell, or a slow unexplained rise in the ITCS accumulator quantities. A rupture is detected by the rapid filling of the ITCS accumulator and/or pressurization of the affected ITCS loop. A rupture is considered anything larger than a pin hole sized breach (> 1.27 mm (0.05 inches)). In response to a rupture of the IFHX and filling of the ITCS accumulator, ISS software will automatically isolate the affected IFHX. However, as seen in Fig. 1, a bleed line exists within the IFHX that prevents full isolation of the IFHX. The bleed line is 0.81 mm (0.032 inches) in diameter. The EATCS operates around 2000kPa (300psi) with a maximum design pressure of 3447 kPa (500psi). The ITCS operates around 190 kPa (28psi) and has a maximum design pressure of 690kPa (100psi). With this high pressure differential it is possible that an IFHX breach can propagate from a micro leak to a rupture scenario. In order to understand the impacts of an ammonia breach on the ISS vehicle and to develop a crew emergency ammonia response strategy, only the rupture case has been analyzed.

### III. Toxicity of Ammonia

As discussed in Ref. 1, ammonia is highly irritating to the eyes, mucous membranes, and respiratory tract. At low levels ammonia acts as an irritant and quickly becomes lethal as levels rise. The National Institute for Occupational Health and Safety (NIOSH) standard for immediate danger to life and health (IDLH) is 300ppm. As will be shown in this paper, the levels of ammonia that could be present in the ISS cabin as a result of an IFHX ammonia leak far exceed this standard. Little data exists on the health effects of ammonia beyond low level exposure. Industry standards dictate immediate evacuation for moderate to high levels of ammonia release. Unfortunately immediate evacuation into a clean zone (area not requiring Personal Protection Equipment (PPE)) is not practical on ISS. NASA medical teams and toxicologists in partnership with Russian specialists at RKK Energia and the Institute of Medico-biological Problems (IMBP) have worked together to define the impacts of ammonia on crew health based on available research as shown in Table 1.

<table>
<thead>
<tr>
<th>mg/M³</th>
<th>Zone</th>
<th>PPM</th>
<th>Ammonia Limit or Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rounded</td>
<td>Rounded</td>
<td>E= Energia; I = IBMP; N = NASA</td>
<td></td>
</tr>
<tr>
<td>21 000</td>
<td>30 000</td>
<td>Skin Blistering within several minutes dermal only contact (E)</td>
<td></td>
</tr>
<tr>
<td>14 000</td>
<td>20 000</td>
<td>Discernable irritation of open skin dermal only contact (E)</td>
<td></td>
</tr>
<tr>
<td>7000</td>
<td>10 000</td>
<td>Faint irritation of open skin dermal only contact (E)</td>
<td></td>
</tr>
<tr>
<td>5000</td>
<td>3520</td>
<td>Rapidly Fatal dose (Henderson, 1927 &amp; Mulder, 1967) (N)</td>
<td></td>
</tr>
<tr>
<td>2500</td>
<td>3520</td>
<td>Deadly concentration (I)</td>
<td></td>
</tr>
<tr>
<td>2500</td>
<td>30-min exposure causes death (Helmers, 1971 &amp; Millea 1989) (N)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1700</td>
<td>2390</td>
<td>Life threatening level (I)</td>
<td></td>
</tr>
<tr>
<td>1720</td>
<td>Coughing (E)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1200</td>
<td>1700</td>
<td>Laryngospasm/airway swelling life threat (Helmers 1971 &amp; Grant) (N)</td>
<td></td>
</tr>
<tr>
<td>7000</td>
<td>1000</td>
<td>ERPG #3 maximum 1-hr exposure without death (N); Hypostasis of lungs possible (I)</td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>1000</td>
<td>Immediate eye injury (Helmers 1971 &amp; Grant 1974) (N)</td>
<td></td>
</tr>
<tr>
<td>350</td>
<td>500</td>
<td>Work without mask impossible (E); Life threatening level and Coughing (I); Heavy irritation of eyes, nose and throat (N)</td>
<td></td>
</tr>
<tr>
<td>280</td>
<td>390</td>
<td>Throat Irritation (I, N)</td>
<td></td>
</tr>
<tr>
<td>360</td>
<td>Work without mask can barely be withstood (E)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>NIOSH Immediate Danger to Life and Health</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Red</td>
<td>200</td>
<td>ERPG #2 maximum 1-hr exposure without serious health effect &amp; work without mask is difficult (E)</td>
<td></td>
</tr>
<tr>
<td>110</td>
<td>Strong eye irritation within one hour (NASA, SMAC vol 1 p 42) (N)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>NRC Emergency 1-hour exposure limit</td>
<td></td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>Begin nose and mouth irritation (E)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| 40    | 60    | Begin eye and upper airway irritation; reflex inspiratory hesitation is
Table 1. Ammonia Effects and Limits in Emergent Acute Exposure

<table>
<thead>
<tr>
<th>Color</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>White</td>
<td>possible (E, I, N)</td>
</tr>
<tr>
<td>50</td>
<td>OSHA max permissible exposure limit (8/hr/d time-weighted avg) (N)</td>
</tr>
<tr>
<td>35</td>
<td>NIOSH max 30 min exposure limit (N)</td>
</tr>
<tr>
<td>Yellow</td>
<td>30 NASA one-hour SMAC (N)</td>
</tr>
<tr>
<td>28</td>
<td>IBMP one-hour MPC (I)</td>
</tr>
<tr>
<td>25</td>
<td>ERPG#1 maximum 1-hr exposure to cause only transient mild symptoms; NIOSH max recommended exposure limit (8/hr/d time-weighted avg) (N)</td>
</tr>
<tr>
<td>14</td>
<td>20 NASA 24-hr SMAC (N)</td>
</tr>
<tr>
<td>7</td>
<td>7 IBMP 24-hr and 7-day MPC (I)</td>
</tr>
<tr>
<td>3</td>
<td>3 NASA 7-day SMAC (N)</td>
</tr>
<tr>
<td>Green</td>
<td>0,7 Odor threshold (E, I, N)</td>
</tr>
</tbody>
</table>

### IV. Current ISS Vehicle Response

The current USOS system control software detects an IFHX leak condition and automatically activates a caution and warning (C&W) toxic alarm on ISS, shuts down intermodule ventilation (IMV) between USOS and IP modules and initiates isolation of the affected IFHX. As previously noted, the IFHX cannot be completely isolated due to the presence of the bleed line. It is possible that a crewmember will smell an ammonia leak before it is detected by the system control software. In that case, a crewmember would manually activate the C&W toxic alarm. The current ammonia response strategy calls for the crew to immediately don oxygen masks, ensure that the C&W toxic alarm has been activated, move as quickly as possible towards the ROS and close the hatch between segments to isolate themselves from the ammonia leakage source. The primary goals of the ISS ammonia leakage response are to evacuate the crew to the ROS as quickly as possible, limit ammonia dispersion into the ROS, and limit ammonia leakage into the ISS atmosphere.

### V. Characterization of the EATCS IFHX Rupture

In order to properly mitigate an ammonia release on board the ISS, it is essential to first characterize the IFHX breach, the flow through the ITCS, and the entry into the cabin. Characterization of the ammonia leak scenario was achieved using three different modeling techniques which include mathematical modeling of the ammonia flow through the thermal control system and out the gas trap completed in 2007 with a follow-on two-dimensional analysis on dispersion through the ISS as well as removal using existing ROS systems in 2012. Computational fluid dynamics (CFD) analysis was then run on the ammonia dispersion through the cabin towards the ROS which was also completed in 2012. For consistency, both the two-dimensional dispersion analysis and the CFD model assumed a 0.05 inch hole is formed in the IFHX, and the hole does not propagate. The 2012 analysis also uses the calculations completed in 2007 for the flow rate of ammonia out of the gas trap. The analysis does not address detailed failure mechanisms, or the likelihood of system failures.

#### A. Modeling Ammonia Release into ISS Atmosphere

In 2007 a mathematical model was developed to predict how much ammonia would be present in the ISS ROS of the ISS by the time the crew is able to isolate the USOS, which at the time was assumed to be approximately 5 minutes, following a EATCS IFHX rupture. The model was also used to determine if an atmosphere could be generated that could present structural (overpressurization) or flammability concerns within the USOS. The scenario that was modeled assumed a mechanical/structural failure of an IFHX causing liquid anhydrous ammonia at high pressure to flow into the ITCS LTL, fully stroking the loops accumulator. The flow of ammonia would then pressurize the ITCS LTL until the weakest part of the loop, the gas trap, fails, after which the water in the loop, as well as the ammonia from the ETCS, would flow into the cabin in an uncontrolled manner as shown in Fig 2.
Several assumptions were made to generate the model, including physical, chemical, and operational assumptions. The physical assumptions of the 2007 model on Ammonia Release into the ISS Cabin were as follows:

1) Nominal cabin pressure of 99.2 kPa (14.4 psia) and temperature of 23.9°C (75 °F)
2) The quantity of ammonia was assumed to be 272.2 kg (600 lbs) at 2688.9 kPa (390 psia), distributed amongst the bellows accumulator and the plumbing between the bellow accumulator and the heat exchanger 136.1 kg (300 lbs), the pump accumulator and the plumbing between the pump accumulator and the heat exchanger 13.6 kg (30 lbs), and heat exchanger and its relevant plumbing 122.5kg (270 lbs)
3) The gas trap of the ITCS would rupture at 1461.7 kPa (212 psig)
4) The size of the rupture in the heat exchanger was expressed as an equivalent hole size, and different diameters of the hole were assumed between 1.27 mm (0.05 inches) and 12.7 mm (0.5 inches)
5) The LTL accumulator’s capacity was 10651.6 cm³ (650 in³), but was initially 75% full
6) The LTL operates in dual loop mode, initially at 124.1 kPa (18 psia), with 62.08 liters (16.4 gallons) of water
7) The internal free volume of the ISS is 636 m³ (2007 projection of assembly complete volume)

These values and assumptions may not hold today at the time this paper is prepared, but were what was available late 2006 / early 2007 when this model was developed.

The assumptions related to chemistry were:
1) Ammonia and water do not interact chemically
2) The entire system is isothermal
3) Once the liquid ammonia/water mixture enters the cabin environment, evaporation of the water and ammonia is instantaneous, but only the evaporation of ammonia contributes to pressure build-up in the cabin
4) Ammonia vapor instantly and evenly distributes throughout the ISS cabin.
5) The operational assumptions of the 2007 model were that there were no operational controls in place:
6) Nitrogen backing pressure from the bellows accumulator was not removed
7) Isolation valves were not closed
8) Caution and warning alarms were not enunciated
9) No automatic software controls were utilized
10) Once ammonia entered the cabin environment, the status of IMV and hatches were unchanged prior to the rupture.

The physical system was modeled as four dependently-coupled subsystems, and it is the flow from one system to the next that was modeled at the subsystems’ interfaces. These four subsystems were:

---

Figure 2. IFHX Rupture Model
1) The bellows accumulator, the pump accumulator, and the plumbing between these components up to the EATCS
2) The EATCS, including the heat exchanger and relevant plumbing
3) The ITCS, including the LTL and its accumulator and the gas trap
4) The cabin volume, including the Pressure Control Assembly (PCA) vent valve (in case the ISS over-pressurizes due to rapid expansion of liquid ammonia to vapor ammonia).

The first interface was between the bellows accumulator and the EATCS, and the flow of liquid ammonia was modeled as liquid flow with friction through the plumbing. The second interface was between the EATCS and the LTL (the IFHX), and the flow of liquid ammonia was modeled as choked liquid flow through an orifice of 1.27 mm (0.05 inch) diameter, representing the rupture of the heat exchanger. The third interface was between the gas trap between the LTL and the cabin environment, and the flow of the ammonia-water mixture was modeled as choked liquid flow through an orifice. The size of the orifice was iteratively calculated such that the pressure in the LTL did not exceed 1461.7 kPa gauge (212 psig), i.e., the hole in the gas trap was sufficiently large enough to maintain 212 psig in the LTL. As liquid ammonia and water exit the gas trap into the cabin environment, the ammonia would undergo a phase-changing throttling process that could cause local pressure effects, but these effects were beyond the scope of this modeling effort. The fourth interface was PCA vent between the cabin environment and space vacuum, and was the flow of ammonia and water was modeled as gaseous sonic flow through an orifice. However, because the focus of this paper is the flow rate of ammonia exiting the gas trap into the cabin environment, cabin pressure effects will not be discussed further.

The flow rate of the water/ammonia mixture flow out of the rupture gas trap was calculated to be 104.3 kg/hr (230 lb/hr) for an equivalent heat exchanger hole size of 1.27 mm (0.05 inch) diameter with the LTL at 1461.7 kPa gauge (212 psig) and the backing pressure inside the heat exchanger was 2688.9 kPa (390 psia). Fig. 3 depicts the timeline of the ammonia release. As the pressure decreases with time, the flow rate also decreases, but that analysis was beyond the scope of the 2007 model. Initially, the flow is primarily water, but as more ammonia flows into the LTL from the heat exchanger, the concentration of ammonia in the mixture increases. For the case of a 0.05 inch hole in the IFHX, the ITCS gas trap breach occurs 10.75 minutes after the IFHX leak initiates.

![Figure 3. Timeline of 0.05" IFHX Rupture](image-url)
B. Two-Dimensional Ammonia Dispersion Assessment

Assessing ammonia dispersion in the ISS cabin at a two-dimensional level assumes that the cabin behaves as two interconnected well-mixed volumes. It is expected that time predictions using this technique are conservative because they neglect the mixing time within each successive module that a more detailed three-dimensional analysis addresses. The two-dimensional analysis uses an ammonia generation rate derived from the analysis of relative timing from interface heat exchanger failure through gas trap failure (as described in the 2007 mathematical model) and the cabin concentration reaching 10000 ppm (1%).

A simultaneous mass balance on each individual segment is conducted for the two-dimensional analysis. The mass balance equations for the USOS and ROS are provided by Eq. (1) and Eq. (2). These equations define the change in contaminant mass as a function of time.

\[
\frac{dM_U}{dt} = \frac{\dot{v}_R}{V_R} M_R - \frac{\dot{v}_U}{V_U} M_U - \sum \eta v M_U + g_U
\]  

(1)

\[
\frac{dM_R}{dt} = \frac{\dot{v}_U}{V_U} M_U - \frac{\dot{v}_R}{V_R} M_R - \sum \eta v M_R + g_R
\]  

(2)

In Eq. (1) and Eq. (2), \( M_U \) is the total mass of contaminant in the USOS, \( M_R \) is the total mass of the contaminant in the ROS, \( V_U \) is the USOS free volume, \( V_R \) is the ROS free volume, \( \dot{v}_U \) is the intermodule ventilation flow from the USOS to ROS, \( \dot{v}_R \) is the intermodule ventilation flow from the ROS to USOS, \( \sum \eta v \) is the removal capacity in the respective segment, \( g_U \) is the generation rate in the USOS, and \( g_R \) is the generation rate in the ROS.

Simultaneous solution of Eq. (1) and Eq. (2) provide an equation for each segment in the form of Eq. (3). In Eq. (3), \( M \) is the total mass of contaminant in the reference cabin volume; \( \alpha, \beta, \) and \( \gamma \) are constants calculated from the segment cabin free volume, ventilation flow, removal capacity, and contaminant generation rate; and \( x_2 \) and \( x_3 \) are integration constants. The integration constants are calculated from the segment free volume, ventilation flow, and removal capacity parameters. Concentration is calculated by simply dividing the contaminant mass by the segment free volume.

\[
M = \alpha + \beta e^{x_2 t} + \gamma e^{x_3 t}
\]  

(3)

If the entire cabin volume is assumed to be well mixed, then the total cabin mass balance equation can be defined more simply as Eq. (4). Derivation of Eq. (4) can be found in Ref. 4. In Eq. (4), \( M \) is the contaminant mass at time, \( t \); \( M_0 \) is the contaminant mass at time equal to zero; \( V \) is cabin volume, \( \sum \eta v \) is the contaminant removal capacity, \( g \) is the contaminant generation rate, and \( t \) is time. However, because ammonia exhibits a gradient, Eq. (4) cannot be readily used. As such, the USOS and ROS are assumed to be separate well-mixed volumes. A composite concentration is then obtained by summing the contaminant mass in each segment and then dividing by the total station free volume.

\[
M = M_0 e^{-\frac{\sum \eta v}{V} t} + \left( g V \sum \eta v \right) \left[ 1 - e^{-\frac{\sum \eta v}{V} t} \right]
\]  

(4)

C. Ammonia Removal Routes

The equipment on board the ISS that possess ammonia removal capacity include the USOS trace contaminant control (TCC) equipment (268 grams), ROS harmful contaminants filter (HCF or Russian acronym FVP) equipment (2 grams), and the humidity control equipment. Under the circumstances of bulk ammonia leakage the TCC and HCF capacity must be assumed to be fully saturated. This leaves ammonia absorption in humidity condensate as the primary removal route for ammonia under bulk ammonia leakage circumstances.

D. Ammonia Removal via Humidity Control Equipment

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. Eq. (5)
shows the basic form solved for liquid phase mole fraction. In Eq. (5), $x$ is the volatile compound liquid phase mole fraction, $y$ is the volatile compound 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. An adjustment, $\alpha$, to the Henry’s Law constant is necessary to account for the 4.4 °C (39.92 °F) heat exchanger operating temperature and liquid phase interactions.\(^6\)

$$x = \frac{y}{C/A + \alpha H/P}$$

(5)

The correlation of Eq. (5) is used to approximate published vapor-liquid equilibrium data at 4.4 °C (39.92 °F).\(^7\) These data are plotted in Fig. 4 and presented in tabular form by Table 2.

![Figure 4. Aqueous Ammonia Vapor-Liquid Equilibrium at 4.4 °C (39.92 °F)](image)
### Table 2. Tabular Vapor-Liquid Equilibrium Data at 4.4 °C (39.92 °F)

The co-current absorption operating curve using Henry’s Law as the equilibrium driving force is used with the Henry’s Law constant equal to $1.60 \times 10^{-5}$ atm-m$^3$/mole at 25 °C.\(^8,9\) This value is adjusted for temperature to the 4.4 °C (39.92 °F) condition by using the vapor pressure ratio temperature dependence estimating technique yielding a value of $8.03 \times 10^{-6}$ atm-m$^3$/mole (0.444 atm/mole fraction).\(^10\) The calculation technique was shown to reasonably predict ammonia loading into cold water up to 15 mole percent and ammonia gas phase concentration up to 83000 ppm using this temperature-adjusted Henry’s Law constant. Once good agreement with the literature vapor-liquid equilibrium data was demonstrated, the Henry’s Law constant was adjusted further to account for reported reactivity with dissolved carbon dioxide thus yielding a final Henry’s Law constant value of 0.0231 atm/mole fraction ($4.17 \times 10^{-7}$ atm-m$^3$/mole).\(^11\) This value is used for calculation purposes. The resulting single pass removal efficiency and condensate loading for the ROS SKV and USOS common cabin air assembly (CCAA) heat exchangers were determined using the co-current adsorption mass balance equation and adjusted Henry’s Law constant.

The performance of humidity control devices to remove ammonia is summarized in Figs. 5, 6, and 7.

![Figure 5. Predicted condensate loading in the ROS SKV as a function of cabin concentration.](image)

<table>
<thead>
<tr>
<th>Mole % NH$_3$</th>
<th>psia</th>
<th>ppmv</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.33</td>
<td>24118.8</td>
</tr>
<tr>
<td>10</td>
<td>0.66</td>
<td>48237.8</td>
</tr>
<tr>
<td>15</td>
<td>1.14</td>
<td>83319.49</td>
</tr>
<tr>
<td>20</td>
<td>1.92</td>
<td>140327.6</td>
</tr>
<tr>
<td>25</td>
<td>3.16</td>
<td>230955.8</td>
</tr>
<tr>
<td>30</td>
<td>5.13</td>
<td>374937.7</td>
</tr>
<tr>
<td>35</td>
<td>7.98</td>
<td>583236.4</td>
</tr>
<tr>
<td>40</td>
<td>11.98</td>
<td>875585.5</td>
</tr>
<tr>
<td>45</td>
<td>17.14</td>
<td>1252716</td>
</tr>
<tr>
<td>50</td>
<td>23.33</td>
<td>1705126</td>
</tr>
<tr>
<td>55</td>
<td>30.15</td>
<td>2203581</td>
</tr>
<tr>
<td>60</td>
<td>37.15</td>
<td>2715192</td>
</tr>
<tr>
<td>65</td>
<td>43.69</td>
<td>3193183</td>
</tr>
<tr>
<td>70</td>
<td>49.56</td>
<td>3622205</td>
</tr>
<tr>
<td>75</td>
<td>54.4</td>
<td>3975948</td>
</tr>
<tr>
<td>80</td>
<td>58.31</td>
<td>4261779</td>
</tr>
<tr>
<td>85</td>
<td>61.62</td>
<td>4503638</td>
</tr>
<tr>
<td>90</td>
<td>64.77</td>
<td>4733863</td>
</tr>
<tr>
<td>95</td>
<td>68.31</td>
<td>4992592</td>
</tr>
</tbody>
</table>

This table provides the tabular vapor-liquid equilibrium data at 4.4 °C, which is crucial for understanding the absorption process and predicting ammonia loading into cold water.
Figure 6. Predicted single pass ammonia removal efficiency provided by the ROS SKV and USOS CCAA. Assessment shows the single pass removal efficiency can be assumed to be constant across the range of cabin concentration between 30 ppm and 10,000 ppm. The concentration reduction calculation takes this into account.

Figure 7. Condensate loading with ammonia for varying condensate collection rates with ammonia at 10,000 ppm in the cabin.

The ROS SKV is predicted to result in condensate loading averaging 361.4 g/kg at a cabin concentration of 10,000 ppm. Note that at 30 ppm, the condensate loading with ammonia is reduced substantially. For the SKV the loading averages 1.08 g/kg condensate over the condensate removal rate range.

E. Two-Dimensional Ammonia Dispersion Prediction
Ammonia dispersion through the ISS cabin when the USOS and ROS are treated as linked, well mixed volumes has been estimated. Figures 8 and 9 provide the estimated dispersion during the first hour of a fluid leak from a 1.27 cm (0.05 inch) equivalent diameter hole. The time to reach 10,000 ppm is also estimated.

![Figure 8. Ammonia dispersion during the first hour of leakage from a 1.27mm (0.05 inch) hole.](image)

![Figure 9. Estimated time to reach 10,000 ppm in the USOS and ROS for varying IFHX hole size.](image)

The two-dimensional analysis indicated that 15 minutes is a critical time period for the crew to recognize that a leak situation exists and retreat to and isolate the ROS from the USOS. Therefore, further two-dimensional analysis of the isolated ROS was conducted.

F. Ammonia Concentration Reduction after Russian Segment Isolation

An additional assessment was conducted that considers ROS isolation from the USOS 15 minutes after the onset of ammonia leakage. This assessment assumes the following:
1) The ventilation between the USOS and ROS is active for 15 minutes after the ammonia begins to leak into the USOS cabin (conservative assumption, as IMV should be shut down by automatic software response upon detection of the rupture).

2) After 15 minutes, the crew has entered the ROS, closed the hatch between the ROS and USOS (physical isolation), and ventilation between the ROS and USOS has been shut down (functional isolation).

3) Ventilation in the ROS remains operational at all times.

4) Ammonia removal in the ROS occurs via absorption into humidity condensate collected by the SKV. For the purposes of analysis, a condensate collection rate equivalent to 6 people is assumed (0.35 liters/hour based on 1.4 liters/person-day production rate). It is assumed that the ISS crew size is six and all crewmembers retreat into the ROS.

5) The USOS and ROS volumes are assumed to be well mixed. Three dimensional gradients are not determined by this level of analysis.

6) No ammonia adsorption onto surfaces is accounted for.

Fig. 10 shows the overall ammonia concentration profile. Within 15 minutes the ROS concentration reaches approximately 4,600 ppm. Fig. 11 shows the first 5 hours after the ammonia leak begins. The peak concentration in the ROS is more easily seen. The concentration in the USOS at 15 minutes is predicted to be approximately 41,460 ppm. After isolating the ROS from the USOS, the ammonia continues to leak into the USOS. Leakage into the USOS continues for approximately 3.75 hours at which time the USOS concentration reaches nearly 637,700 ppm.
Figure 11. Calculated ammonia concentration profile for the first 5 hours after leakage begins. The ROS is isolated from the USOS 15 minutes after leakage begins

No more ammonia enters the ROS after it is isolated from the USOS. As humidity condensate is collected by the ROS SKV unit, ammonia is removed in the condensate via absorption. This is the primary removal method considered for the assessment. It is recognized that ammonia may adsorb onto surfaces in the ROS leading to further concentration reduction. However, that phenomenon is very difficult to characterize and is not considered by this assessment. Neglecting the surface adsorption phenomenon, however, contributes to the present assessment’s conservatism.

After approximately 25 hours, the ammonia concentration is predicted to reach 500 ppm if a 6-person condensate collection rate is sustained. Fig. 12 shows the predicted concentration reduction below 500 ppm. At a sustained 6-person humidity condensate collection rate, it is predicted that the concentration in the ROS will be reduced to 300 ppm in approximately 30 hours after the ROS is isolated from the USOS. The concentration is predicted to reach 100 ppm 43 hours after ROS isolation. The ultimate goal of reaching 30 ppm is reached 56 hours after isolation.

The results presented depend on the sustained humidity condensate rate and other variables such as surface adsorption phenomena.
Figure 12. Calculated ammonia concentration profile showing the range below 500 ppm.

Humidity collection rate can affect the time required to reduce the ROS cabin concentration. A more detailed evaluation beginning at a 300 ppm cabin concentration is presented by Fig. 13. Humidity condensate collection at a 3-person rate or higher is predicted to reduce the ammonia concentration most effectively from the 300 ppm cabin concentration condition. Crew members may need to use personal protective equipment and monitor the ammonia concentrations for 12 and up to 24 hours for a 300 ppm ROS cabin concentration condition. If concentrations >300 ppm exist in the ROS, then more time will be required as indicated by Figs. 10, 11, and 12.
To resolve aspects of conservatism associated with the two-dimensional analysis, it is necessary to also consider the CFD techniques and tools when formulating an ammonia response strategy.

G. Computational Fluid Dynamics (CFD) Modeling: Ammonia Spread through the ISS Atmosphere

Using the 2007 mathematical model on ammonia release into the ISS cabin, a CFD model was developed to describe the migration of ammonia throughout the ISS. Figure 14 shows the three dimensional (3D) model of the ISS modules that was used for the analysis. Four cases were analyzed using this model. Case 1 represents the baseline case, the ISS ventilation system is modeled with the current automatic toxic alarm software response: USOS and IP IMV off including the IMV flow between ROS and USOS. Case 2 models the current toxic alarm software response with the addition of the hatch closure 5 minutes after the gas trap rupture between the ROS and USOS segment. It is important to note that for Case 2, computations are performed for the RS only once the hatch between segments is closed. Case 3 modeled all of the ISS ventilation off (both IMV and internal cabin fans), making the flow of the ammonia through the gas trap the only motive force. Finally, in Case 4 the current automatic toxic alarm software response is modeled with the addition of the Node 1 cabin fan being turned off. It was theorized that the Node 1 cabin fan promotes flow of ammonia from the USOS to ROS.

For the model, it is assumed that the breach of the ITCS occurs at the gas trap located in Lab Port 6 location (Aft on Port side). This location is considered conservative in that it represents the worst case scenario concerning ROS ammonia contamination.
For Case 1, which models the current vehicle response to a toxic alarm, a strong ammonia jet is formed in the U.S. Laboratory immediately after gas trap failure. As the volumetric flow of ammonia/water mixture is about 40 cfm, the effect of the ammonia jet on the flow structure is comparable with the effect of the airflow from the common diffuser. Ammonia concentration distributions are presented in Fig. 15a for the instant of 5 minutes and Fig 16a for the instant of 15 minutes from the gas trap rupture. Volume-averaged ammonia concentration in the PMA reach 10,000 ppm at 15 minutes post gas trap rupture. An ammonia concentration of about 1000 ppm is achieved in Soyuz 1, and Soyuz 2 averages about 60 ppm at the same instant. The ventilation scheme in the ROS is designed such that it pulls air from the core modules and ducts it to the appending modules. For this reason the Soyuz 1 module has a higher concentration of ammonia than its preceding module, MRM 1. The current toxic alarm response, as modeled in Case 1, is therefore insufficient in limiting contamination of the ROS.

If the ROS is isolated 5 minutes after the gas trap rupture, as modeled in Case 2, the situation with the ammonia dispersion over the ROS seems to be more favorable. Only about 2 g of ammonia penetrate to the ROS in the initial 5 minute period. At this instant the peak value of ammonia concentration achieved in PMA is about 300 ppm (see Fig. 17b). Once the hatch is closed and the ROS is isolated from the ammonia source, the long process of air mixing and equalization begins. After about 120 minutes, the ammonia fraction in the ROS is about 14 ppm. Though ammonia response strategy calls for immediate evacuation of the USOS upon detection of a leak, it is not possible to know for certain how long it will take crew to respond due to unforeseen events (crew injury, crew activity/location at the time of the event, etc...).

Complete shutdown of ventilation in the ISS immediately after the IFHX breach is detected, as modeled in Case 3 (see Fig. 15b), could allow for the ROS to remain uncontaminated for about 12 minutes post rupture, but after that, diffusion leads to gradual penetration of ammonia to PMA, FGB and other Russian modules. At the instant of 15 minutes post gas trap rupture, volume-averaged ammonia concentration in PMA reach about 65 ppm (see Fig. 17c), and it grows rapidly. Soyuz 1 and 2 remain clean over the 15 minute span computed. It could be concluded that if ammonia transport is due to diffusion only, the ammonia-rich cloud propagates relatively slow.

A recommended way to reduce the ammonia content in the ROS, if a full ISS ventilation shutdown is not practical, is to switch off the Node 1 internal ventilation (Case 4). If Node 1 ventilation is switched off immediately after the IFHX breach is detected, ammonia concentration in the ROS is noticeably lower. At 15 minutes post rupture, the volume-averaged ammonia concentration in PMA is about 2000 ppm. A much reduced ammonia concentration of about 100 ppm is achieved in Soyuz 1, and a concentration of about 3 ppm in Soyuz 2.
Figure 15. NH3 content at ISS aft-forward midplane computed at the instant of 5 min from the start of NH3 leakage into the cabin (a) Cases 1 and 2, (b) Case 3, (c) Case 4.
Figure 16. NH3 content at ISS aft-forward midplane Y = 0 computed at the instant of 15 min from the start of NH3 leakage into the cabin (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

Figure 17. Volume-averaged ammonia concentration profile in PMA: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.
VI. Ammonia Response Strategy and Future Mitigation

The CFD and two-dimensional dispersion analysis completed in 2012 add rigor to the analysis completed in 2007. Within the key initial response timeframe of 15 min considered, the CFD analysis shows that the flow of ammonia towards the ROS is slower than what is predicted assuming a well mixed volume, however the localized concentrations can be extremely high and vary greatly within and between modules. The CFD analysis also reveals the affects of ventilation on the flow of ammonia and highlights areas where ventilation is aiding the flow of ammonia to the ROS and causing contamination of the crew escape vehicles. These ventilation effects are shown to be incredibly important during the initial response to the leak. Analysis also shows that the ammonia removal in the ROS via absorption into humidity condensate collected by the CKB is relatively small compared to the amount of ammonia that could enter the ROS.

Using this analysis, the ISS Emergency Response team is working to update the ammonia response strategy to improve both crew and vehicle safety. The crew response has been updated to send the crewmembers directly to their Soyuz vehicles as quickly as possible post hatch closure between the Russian and US segment. The goal of this response change is to stop flow of ammonia into the crew’s Soyuz vehicles as well as make a best effort to establish a clean environment for crew within the vehicle.

Some of the vehicle software changes that are in-work include powering off of the Node 1 Cabin Fan which was shown in Case 4 of the CFD model to greatly reduce the flow of ammonia into the ROS. Work has also been initiated to power off all Russian fans in order to stop the flow of ammonia into the Soyuz vehicles. The Russian fans will be re-powered after 30 minutes in order to evenly disperse the ammonia throughout the ROS, once crew is safely established in their Soyuz vehicles. If ammonia measurements within the Soyuz are low enough for doffing of PPE (100ppm and decreasing or < 30 ppm) crewmembers, with direction from the ground, will consider re-ingressing the ROS. Per analysis, the ROS ventilation system will take about 2 hours to disperse the ammonia evenly throughout the segment. Once dispersion is considered to be complete, ROS fans will be unpowered to halt the circulation of ammonia within the ROS, and a crewmember will re-open the Soyuz hatch enough to quickly sample the module air. If ammonia levels are below PPE doffing limits, the crewmembers can re-ingress the ROS. As the analysis shows, the ROS CKB can reduce ammonia levels with a 6 crewmember latent load within 24 hours. If a clean zone can’t be established within the Soyuz considering available PPE, then crewmembers along with ground support, will initiate an undock and return.

The ISS Program has also initiated funding to design, manufacture, and launch ammonia specific scrubbing systems for both the Soyuz vehicles and the Russian Segment. Recovery of the USOS and IP modules is also considered in future work.

References

8Agency for Toxic Substances and Disease Registry. Toxicology Profile of Ammonia. ATSDR 1990a.