Numerical Study of Ammonia Leak and Dispersion in the International Space Station

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Release of ammonia into the International Space Station (ISS) cabin atmosphere can occur if the water/ammonia barrier breach of the active thermal control system (ATCS) interface heat exchanger (IFHX) happens. After IFHX breach liquid ammonia is introduced into the water-filled internal thermal control system (ITCS) and then to the cabin environment through a ruptured gas trap. Once the liquid water/ammonia mixture exits ITCS, it instantly vaporizes and mixes with the U.S. Laboratory cabin air that results in rapid deterioration of the cabin conditions. The goal of the study is to assess ammonia propagation in the Station after IFHX breach to plan the operation procedure. A Computational Fluid Dynamics (CFD) model for accurate prediction of airflow and ammonia transport within each of the modules in the ISS cabin was developed. CFD data on ammonia content in the cabin aisle way of the ISS and, in particular, in the Russian On-Orbit Segment during the period of 15 minutes after gas trap rupture are presented for four scenarios of rupture response. Localized effects of ammonia dispersion and risk mitigation are discussed.

I. Introduction

MANAGING cabin air quality is a key issue for space exploration missions. To ensure safe and comfort conditions during nominal operation of the International Space Station (ISS) it is necessary to obtain a balance between the generation and removal of contaminants, in particular, ammonia.[1] Small amount of ammonia generated in the cabin atmosphere (300 mg/day per person due to metabolic process[2]) is successfully scrubbed by several ISS subsystems.[3]

Management of off-nominal situations on-board the International Space Station (ISS) is important to ensure its continuous operation. A possible ammonia release into the cabin atmosphere is related with the active thermal control system (ATCS)[4] operation. Ammonia assists with heat exchange in ATCS currently in the U.S. Laboratory of the ISS. ATCS is a combination of two systems, the external active thermal control system (ETCS), and the internal active thermal control system (ITCS). The ETCS and ITCS are closed-loop systems which utilize liquid ammonia and water, respectively, as heat-transfer fluids. There is approximately 272 kg (600 lbs) of liquid ammonia in the ETCS circulating through interface heat exchangers (IFHX) transferring heat from the ITCS water lines[1]. ETCS ammonia pressure is 390 psia, while ITCS water pressure is 18 psia. High-pressure ammonia could enter the internal compartments by leaking from the external loops to the internal loops, and then into the cabin atmosphere, in case of IFHX breach. Hence the ATCS is a possible source of ammonia in case of IFHX breach.

Scenarios and mitigation of an ammonia release on board of the ISS are discussed in Ref. 1. If the leak occurs, a micro-leak, a moderate leak, and a catastrophic rupture can exist in ATCS. A micro-leak or a moderate-leak can occur through small cracks in the IFHX. In this case trace contaminant control systems along with the condensing heat exchangers on the ISS should be able to maintain cabin atmosphere concentrations, though noticeable ammonia odor can occur for some time. A response to an ammonia release event detected by crew senses or a detector should be through the steps of isolation, power shutoff, and ventilation airflow cessation. In this case crew will have to don portable breathing apparatus, evacuate to the Russian On-Orbit Segment (ROS) and isolate the U.S. On-Orbit Segment (USOS).

The limits of ammonia concentration in the cabin atmosphere are quite low.[2] One-hour Station maximum allowed concentration (SMAC) is 20 mg/m^3. It is safe to doff the ammonia respirator. The concentration of 65 mg/m^3 is safe to doff the respirator if the crew wants to and if the concentration is decreasing with time. The concentration of 200 mg/m^3 is the Immediate Danger to Life and Health (IDLH), and the most current concentration that the ISS crew will evacuate at with existing scrubbing capabilities. The concentration of 800 mg/m^3 is the upper limit certified for the ammonia respirator. It is evident that ammonia concentration in the cabin locally (USOS) will rise quickly based on the amount leaked in. However, there are many questions about ammonia dispersion in the whole station and mostly to the ROS where the crew is planned to evacuate. The goal of the study is to find out the evolution of the NH_3 distributions in the ISS cabin atmosphere in case of a catastrophic rupture using a Computational Fluid Dynamics (CFD) model. The computations have been performed with the ANSYS FLUENT 12.1.4 CFD software.[5]

II. Computational Model

A. Gas trap rupture modeling

The catastrophic rupture scenario model used in the current computations is as follows.

It is assumed that liquid ammonia starts to flow through a "pin-hole"-sized breach of the IFHX with the diameter of 0.05". For this value of IFHX orifice diameter the flowrate of ammonia is equal to 72.5 kg/hr. After the IFHX breach pressure in the ITCS is increased continuously until the burst pressure of the gas trap is reached and a gas trap breach occurs. It is assumed that the gas trap rupture happens 10.75 minutes after the IFHX breach occurs. The gas trap location is assumed at rack P6 in the U.S. Laboratory.

It is assumed that upon a verified alarm of IFHX breach, the USOS IMV ventilation is shut down within 5 minutes. The interval between the IMV shutting off and the gas trap rupture is about 6 minutes that seems to be enough for the airflow to change from one stable pattern to another. Hence CFD modeling starts at the gas trap rupture moment with the initial flow field without IMV.

Starting from the instant of 10.75 minutes, ammonia/water mixture flows from the ITCS loop into the cabin environment through a ruptured gas trap. It is assumed that once the liquid water/ammonia mixture exits the ITCS, it instantly vaporizes, and the resulting gas is supplied to the cabin through an opening in the panel of the U.S. Laboratory rack P6.

The ratio for liquid water and ammonia in ITCS loop is computed using the following relation:

$$y_{NH_3}(t) = \frac{\dot{m} \cdot t_{IFHX\_breach}}{\dot{m} \cdot t_{IFHX\_breach} + m_{water\_ini}} \tag{1}$$

where y_{NH_3} is the mass fraction of ammonia at time (t), $\dot{m}$ = 72.5 kg/hr is the mass rate, m_{water_ini} = 62.1 kg is the initial mass of water in the ITCS loop. This value of mass fraction given by the relation (1) is assumed as the inlet value at the panel opening assumed to be the ammonia inlet section for the CFD modeling. The ammonia mass fraction evolution is plotted in Fig. 1. Note that the ammonia/water mixture release into the cabin starts at time instant of 10.75 min.

Two additional simplifications of the model should be mentioned. First, ammonia removal possibilities of the Station are neglected for the analyzed time frame. Some ISS modules have air conditioning unit which is able to collect the vapor and condensate, so that small amount of NH_3 could be removed from the atmosphere in these modules[1], but the amount of ammonia removed is very small as compared with the mass released during the catastrophic rupture. The ammonia production due to crew metabolic respiration is neglected as well.

Another simplification is that crew member movement that could add some momentum and change the flow field is neglected, as it is supposed to be a local effect without strong impact on the global velocity distribution.

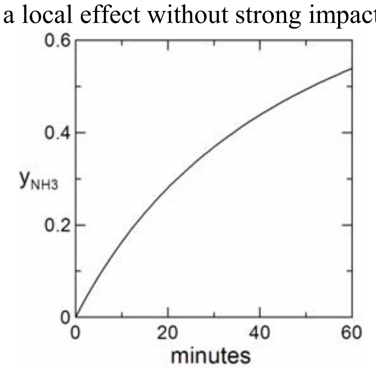

Figure 1. Ammonia concentration evolution in the ITCS loop; this curve defines the mass of ammonia supplied to the cabin at each time step.

B. Cabin Aisle Way Geometry Model and Airflow Boundary Conditions

The 3D geometry model of the ISS aisle way adopted for the present CFD analysis of the cabin ventilation is illustrated in Fig. 2. The CFD model takes into account the cabin aisle volume only. The model of the ROS consists of the following modules: the Service Module (SM), the Functional Cargo Block (FGB), Pressurized Mating Adapter (PMA), Mini Research Module 1&2 (MRM 1&2), Multipurpose Laboratory Module (MLM), Progress 1&2, Soyuz 1&2. The USOS includes Node 1, the U.S. Airlock, Node 3 with Cupola, Pressurized Multipurpose Module (PMM), the U.S. Laboratory, Node 2, Columbus, and the Japanese Pressurized Module (JPM) with the Japanese Logistics Module (JLP).

The air density is computed using the ideal gas law for an incompressible flow. In this form, the density depends only on the operating pressure and not on the local relative pressure field.

The inlet/outlet velocity boundary conditions are set with the uniform inlet velocity approximation adopted for each inlet diffuser. The velocity magnitude for each diffuser is defined by a corresponding volumetric flow rate and an effective area of the diffuser. As well, the uniform velocity boundary condition is imposed for each return grille, except the return grille in the Service Module, where the pressure outlet boundary condition is set. A no-slip boundary condition is imposed on all of the solid ISS surfaces. The details of the problem formulation for the ISS airflow modeling the core complete ISS configuration when all the ISS modules are taken into account could be found in Ref. 6.

The schematic of the ISS flow rates (in cubic feet per minute, cfm) adopted for the baseline case, Case 1, is given in Fig. 3. The flow through boundaries of the computational domain (diffusers and return grilles, treated with proper boundary conditions) is marked by black, while the IMV hatch flow is marked by red. All interior hatches between ISS modules are assumed to be open. As computations are performed for the period after that the IFHX breach is detected, IMV flow in the USOS is switched off.

Contrary to the USOS, in the ROS the IMV ventilation is on. Note that there is a diffuser in the middle of PMA on port side closed with a soft cover. Since Node 3 IMV is closed, the IMV flow leakage from the Service Module was assumed at this diffuser. The diffuser was considered as an outlet with the flow rate of 20 cfm.

In Case 2 the hatch between Node 1 and PMA (between ROS and USOS) is closed at the elapsed time of 5 minutes from the start of ammonia release (the moment of gas trap rupture). Note that for Case 2 for the period after hatch close, computations are performed for ROS only. Removal of the USOS computational domain starting from 5 min allowed to perform computations two times faster.

In Case 3 all the ISS ventilation is switched off (both IMV and internal).

Finally, in Case 4 the Node 1 internal ventilation is switched off, while other internal ventilation systems are operating, as well as the IMV in the ROS, the same as in Case 1.

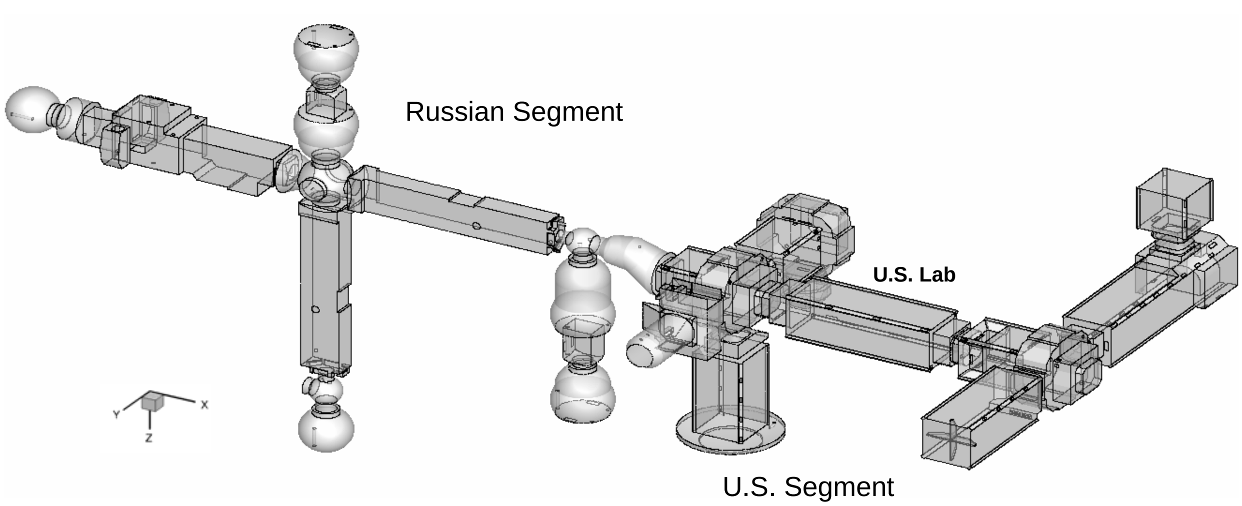

Figure 2. Geometry model used for CFD Study of ammonia dispersion.

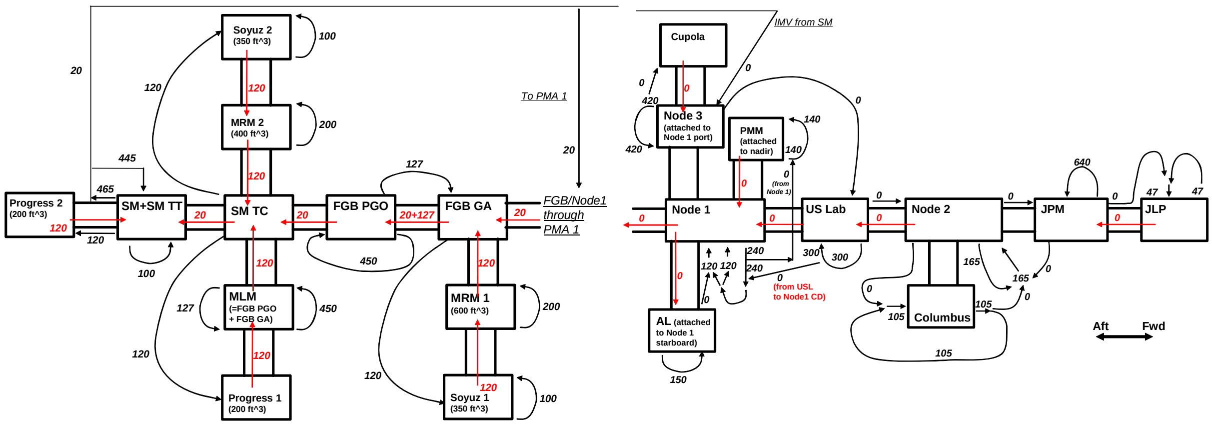

Figure 3. Flow rates adopted for ISS ventilation computations in the basic Case 1.

C. Ammonia Transport Problem Formulation

Unsteady NH_3 transport equations were solved coupled with the unsteady airflow problem. The steady-state air velocity field was used as the initial field for each particular case. For Cases 1 and 2 the same velocity field corresponding to the switched off IMV ventilation was used. For Case 4 this initial velocity field was recalculated to provide the absence of ventilation in Node 1. For Case 3 zero initial velocities were set for the entire cabin.

Zero initial ammonia concentration was set. Initial cabin temperature of 75°F was set. Initial cabin pressure was 14.4 psia. Boundary conditions for the ammonia transport problem were as follows. The only source of ammonia is the mass supplied from the gas trap to the under-panel space, and then to the U.S. Laboratory cabin via the panel opening. The panel opening is assumed to be a rectangular hole approximately 20 by 4 inches (with the area of 0.7 ft^2).

In the CFD model the water/ammonia mixture of 72.5 kg/hr is supplied to the cabin via the panel opening. The value of ammonia mass fraction is set according to relation (1). The inlet density was varied in time to set the correct ammonia mass supplied to the cabin. The area of the opening assumed corresponds to inlet velocity of about 50-60 ft/min, depending on the mixture density. The inlet boundary condition at the panel opening was set by means of a specialized ANSYS FLUENT User Defined Function (UDF).

The inlet ammonia boundary conditions on the diffuser surfaces in all the ISS modules were set by means of an ANSYS FLUENT UDF as well. The UDF defines the inlet ammonia boundary conditions on the diffuser surfaces using ammonia values averaged over the correspondent outlet sections. Some details of the integrated model for contaminant (carbon dioxide) transport in the ISS cabin can be found in Ref. 6.

D. Computational Aspects and Turbulence Modeling

The computational grid generated for the PFE discharge CFD modeling is fully unstructured with tetrahedral mesh elements. The tetrahedral grids were created using the GAMBIT 2.4.6 generator.[8] The grids are clustered to the solid walls and to the diffusers. As well, clustering was performed for the region near the ammonia exhaust surface in the U.S. Laboratory.

The FLUENT solver, being face-based, supports polyhedral cells.[5] Advantages that polyhedral meshes have shown over some of the tetrahedral or hybrid meshes is the lower overall cell count, almost 3-5 times lower for unstructured meshes than the original cell count, keeping the same spatial accuracy.

Conversion of the initial tetrahedral grid to polyhedral one was performed in FLUENT, see Ref. 5 for details. The clustering of the grids to the walls and to the diffusers was kept during the conversion procedure. The final polyhedral grid consisted of about 6,900 thousand cells (that corresponds to more than 34 million nodes).

The Reynolds-Averaged Navier-Stokes (RANS) approach was employed. The RANS-based modeling approach greatly reduces the required computational effort and resources, and is widely adopted for practical engineering applications. For the ISS ventilation case, a comparison of the Columbus experimental data with the results of 3D RANS computations as well as with the accurate Large Eddy Simulation computations prove that RANS modeling is quite accurate regarding to air ventilation velocity field.[9]

The realizable k-ε model[10], with the standard wall functions[11], was used for computations. The wall distance of a cell centre adjacent to a solid wall measured in wall units, y_p^+, ranged from 10 to 50 over the majority of the solid walls. The inlet turbulence intensity was taken as 10% for all the diffusers while the inlet ratio of the turbulent to molecular viscosity, ν_{tur}/ν, was varied from diffuser to diffuser to ensure that the inlet-jet effective Reynolds numbers, $Re_{eff} = V_{in}L_s/(\nu+\nu_{tur})$, are within the range from 200 to 300. Here V_{in} is the inlet velocity value, and L_s is the inlet length scale (the diffuser width).

The governing equations for conservation of mass, momentum, and turbulence characteristics were solved using the unsteady segregated pressure-based solver.[7] The SIMPLEC pressure-velocity coupling scheme was used. The second-order upwind spatial discretization scheme was used, both for the momentum and the k-ε model governing equations. The second-order pressure interpolation scheme was employed. The under-relaxation factors of 0.8 were set for the pressure and turbulence characteristics, while for the momentum the under-relaxation factor was 0.9.

The second order implicit transient formulation was used. For each case the sample of 15 minutes (900 seconds) from the instant of the gas trap rupture was computed. The time step was varied. Over the initial 20 steps the extremely small time step of 0.005 s was used to resolve rapid changes in the airflow immediately after the start of the ammonia discharge. Then the time step was increased gradually up to 1 s for the final period when the changes in the U.S. Laboratory airflow are slow.

For numerical simulation acceleration, parallel computations were performed using eight processes of a LINUX-based cluster.

III. Results and discussion

The first problem to be discussed is the air exchange between the USOS and ROS though the IMV ventilation is switched off. The flow field in the U.S. Laboratory is illustrated in Fig. 4 where instantaneous streamtraces issued from the section used for ammonia/water mixture modeling are given for Case 1. 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 significant.

As the crew is planned to be evacuated to the ROS after the gas trap rupture, the goal is to reduce ammonia dispersion to the ROS. However it is visible in Fig. 4 that though the total inter-module flow through the open hatch is small (it is not equal to zero as the excess mass discharged into the U.S. Laboratory is distributed all over the Station), some pathlines penetrate to the neighboring Node 1 in the aft direction and further to the ROS. Air rich with ammonia spreads also in the forward direction, to Node 2 and attached modules.

Another illustration of the inter-module flow to the ROS is shown in Fig. 5. Pathlines issued from the Node 1 linear diffusers and Node 1 starboard diffuser (aft side) illustrate air exchange between the neighboring modules. Strong airflow from the USOS to the ROS is detected (Fig. 5b). It could be concluded that stopping IMV ventilation is not enough to eliminate ammonia dispersion to the ROS.

This conclusion is confirmed by the ammonia concentration distributions presented in Fig. 6a for the instant of 5 minutes and Fig 7a for the instant of 15 minutes from the gas trap rupture. Volume-averaged ammonia concentration in PMA in basic Case 1 reaches 10,000 mg/m^3 at the instant of 15 minutes. As well high ammonia concentration of about 1000 mg/m^3 is achieved in Soyuz 1, and NH_3 concentration in Soyuz 2 is about 60 mg/m^3 at the same instant.

If ROS is isolated at the instant of 5 minutes from gas trap rupture, the situation with the ammonia dispersion over the ROS seems to be more favorable. Even in the basic case of IMV shutdown with the internal ventilation on, only about 2 g of ammonia penetrate to the ROS during initial period of 5 minutes. The peak value of ammonia concentration achieved in PMA is approximately 300 mg/m^3 (see Fig. 8c). At the instant of hatch closing the ROS air mixing starts that seems to be a long process After complete mixing, the ammonia fraction in the ROS of 140 m^3 will be about 14 mg/m^3. In this case the ROS hardware seems to be able to clean the ROS to acceptable levels, and probability of maintaining crew safety and ISS operations after the catastrophic ammonia release is higher.

Complete shutdown of ventilation in the ISS immediately after IFHX breach is detected could allow keeping the ROS clean during the period of about 12 minutes, but after that diffusion leads to gradual penetration of ammonia to PMA, FGB and other Russian modules. At the instant of 15 minutes volume-averaged ammonia concentration in PMA in Case 3 is about 65 mg/m^3 (see Fig. 8c), and it grows rapidly. The ammonia concentration in Soyuz 1 and 2 remains low over the whole sample of 15 minutes computed.

A recommended way to reduce the ammonia content in the ROS if it is not possible to isolate the ROS quickly is to switch off the Node 1 internal ventilation (Case 3). If Node 1 ventilation is switched off immediately after IFHX breach is detected, ammonia concentration in the ROS is noticeably lower. At the instant of 15 minutes volume-averaged ammonia concentration in PMA in Case 4 is about 2000 mg/m^3. As well reduced ammonia concentration of about 100 mg/m^3 is achieved in Soyuz 1, and NH_3 concentration in Soyuz 2 is about 3 mg/m^3 at the same instant.

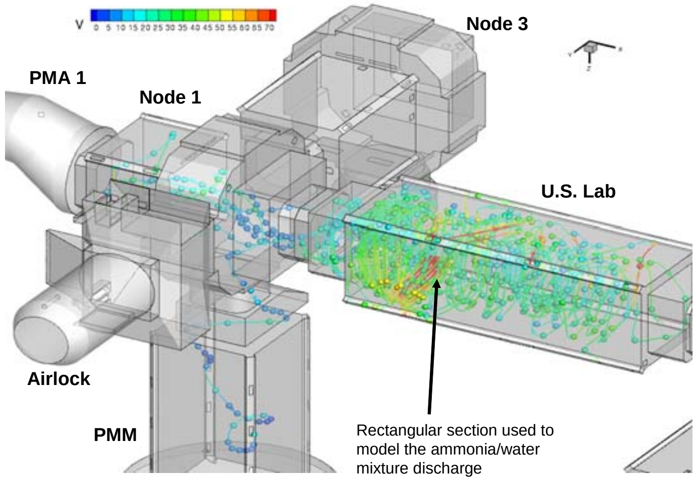

Figure 4. Pathlines colored with velocity magnitude issued from the U.S. Laboratory rack surface section used for ammonia/water mixture release modeling (Case 1).

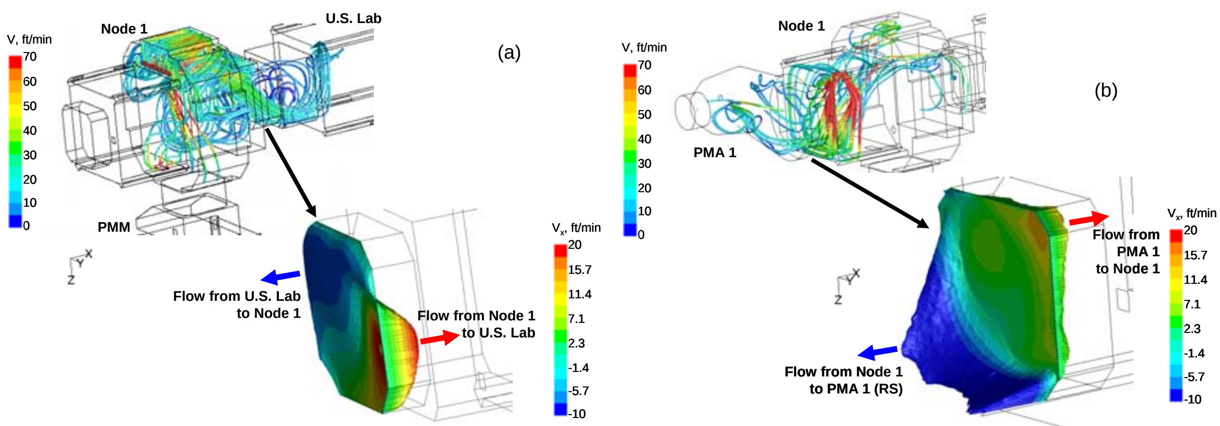

Figure 5. (a) Pathlines issued from the Node 1 linear diffusers and velocity distribution over Node1/U.S.Lab hatch. (b) Pathlines issued from the Node 1 starboard diffuser (aft side) and velocity distribution over PMA1/Node1 hatch. All data are presented for Case 1.

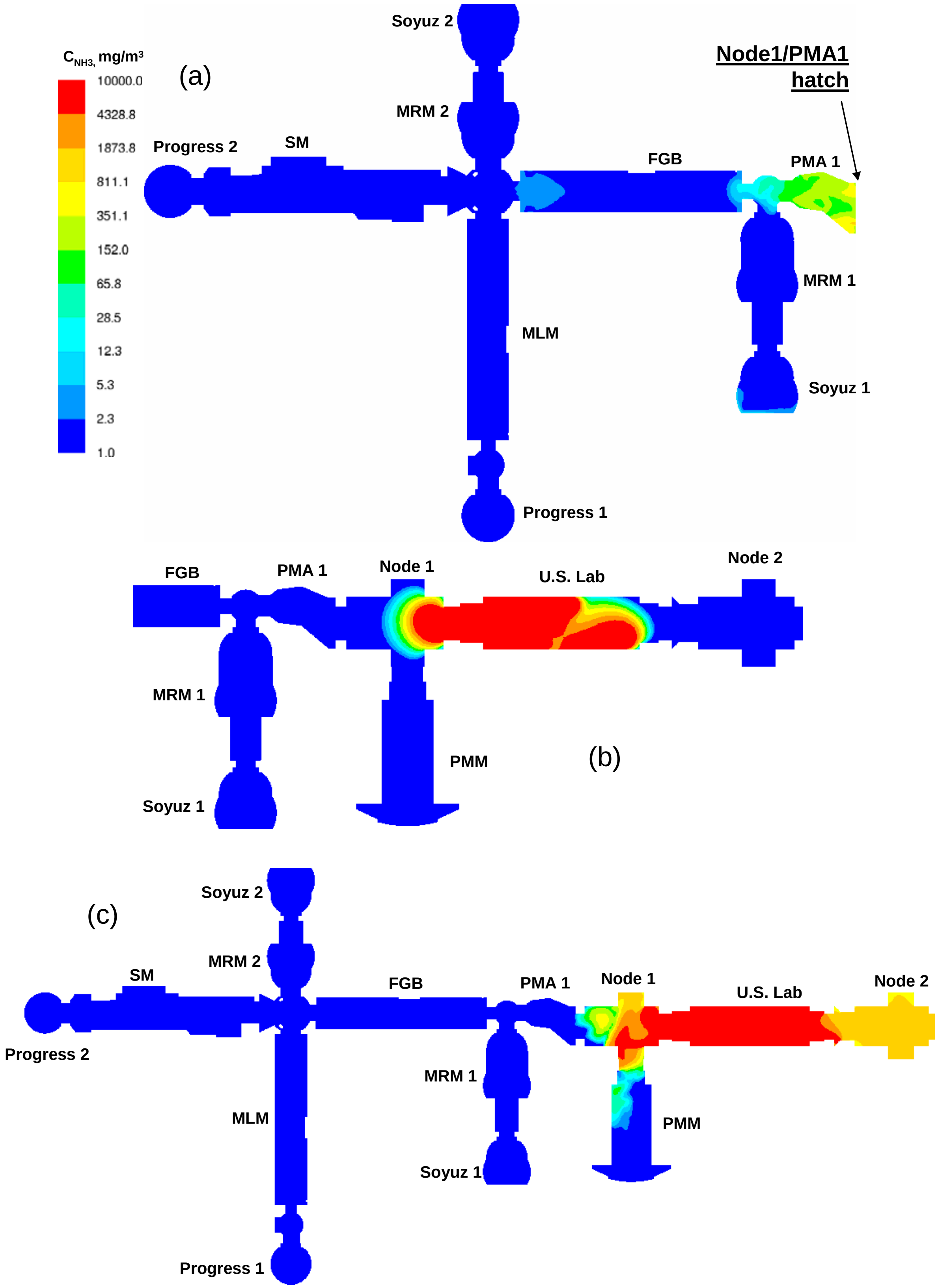

Figure 6. NH_3 content at ISS aft-forward midplane Y = 0 computed at the instant of 5 min from the start of NH_3 leakage (15.75 min from the HX Breach). (a) Cases 1 and 2, (b) Case 3, (c) Case 4.

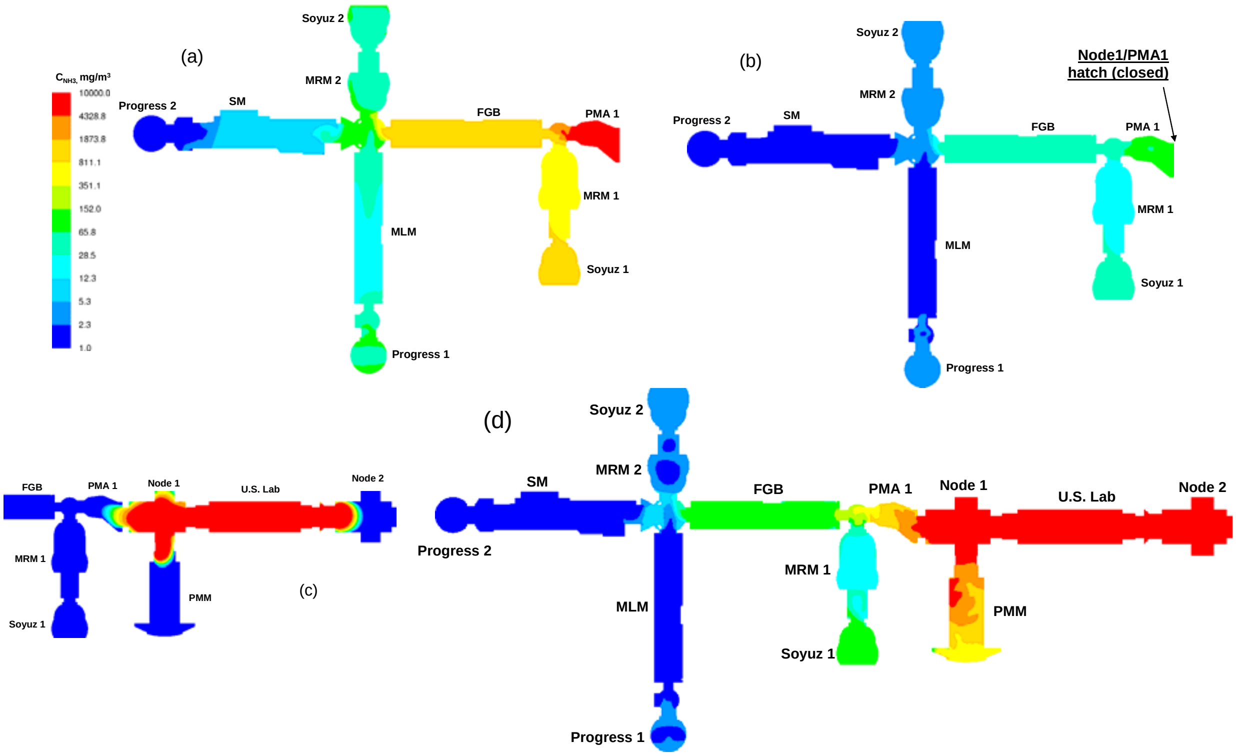

Figure 7. NH_3 content at ISS aft-forward midplane Y = 0 computed at the instant of 15 min from the start of NH_3 leakage (25.75 min from the HX Breach). (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

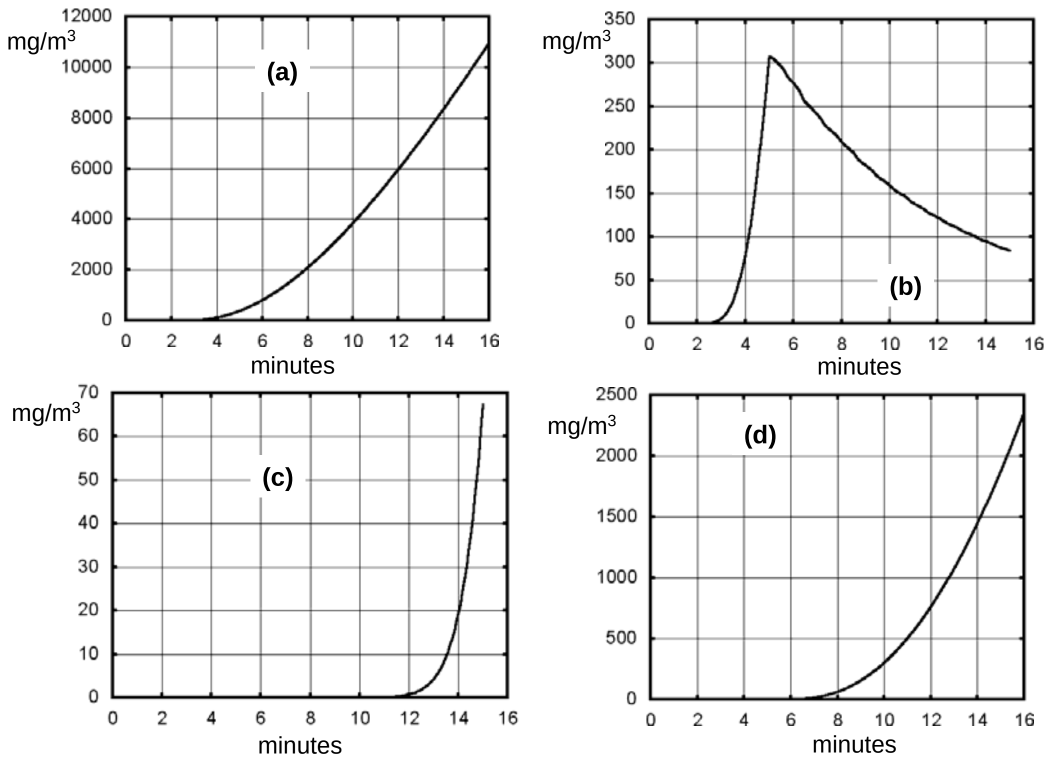

Figure 8. Volume-averaged ammonia concentration evolution in PMA: (a) Case 1, (b) Case 2, (c) Case 3, (d) Case 4.

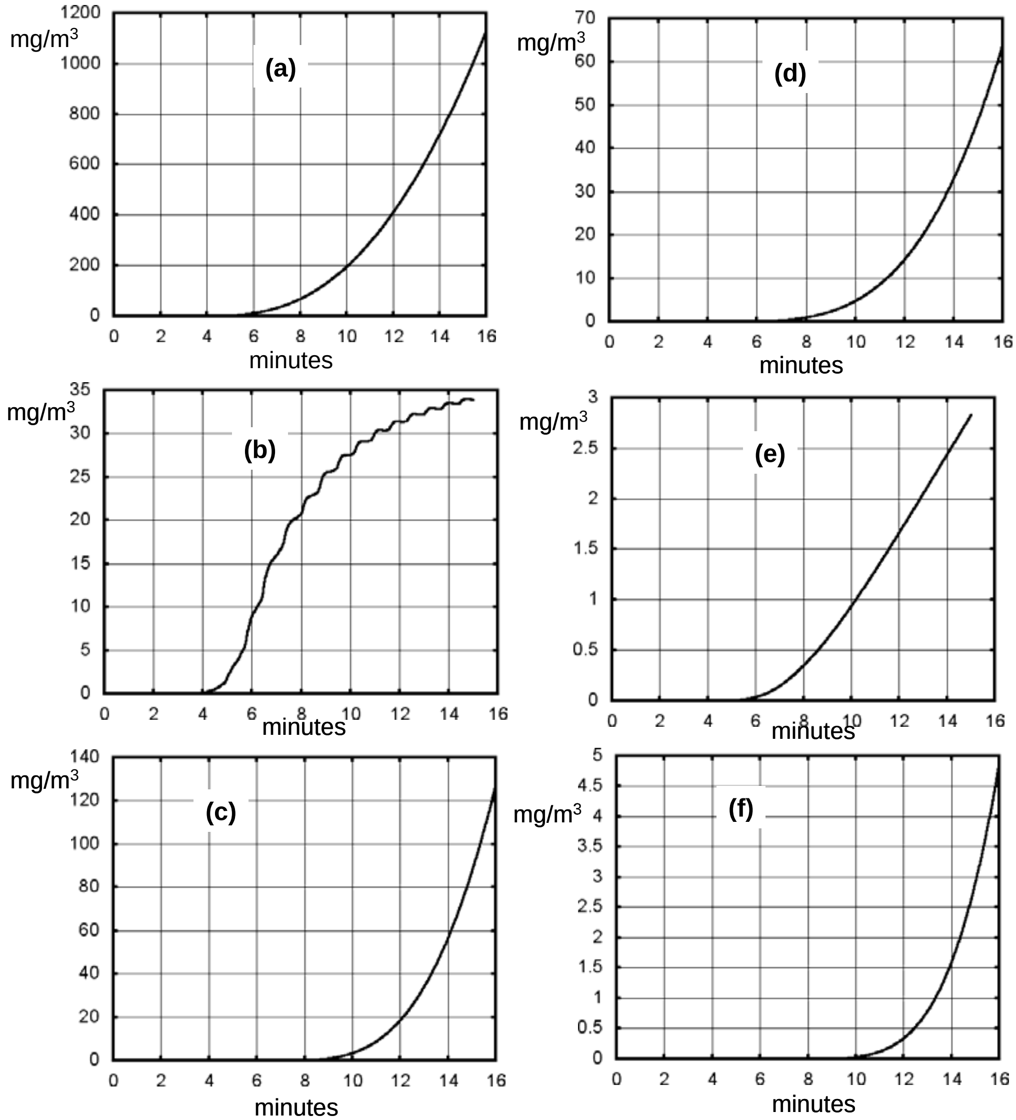

Figure 9. Volume-averaged ammonia concentration evolution in (a,b,c) Soyuz 1 and (d,e,f) Soyuz 2: (a,d) Case 1, (b,e) Case 2, (c,f) Case 4; for Case 3 ammonia concentration is equal to zero during the period considered.

IV. Conclusion

Ammonia discharge process in the U.S. Laboratory module after IFHX breach was numerically simulated using the CFD technology. A detailed analysis of the NH_3 content in the cabin aisle way of the ISS and, in particular, in the ROS during the period of 15 minutes after gas trap rupture was performed for four scenarios of rupture response.

It was shown that if the ROS is not isolated during the period considered, high ammonia concentration of about 1000 mg/m^3 is achieved in Soyuz 1, while NH3 concentration in Soyuz 2 is about 60 mg/m^3. If Node 1 ventilation is switched off immediately, ammonia concentration in the ROS is noticeably lower. Complete shutdown of ventilation in the ISS could allow keeping the ROS clean during the period of about 12 minutes, but after that diffusion leads to gradual penetration of ammonia to FGB and other Russian modules. If ROS is isolated at the instant of 5 minutes from gas trap rupture, approximately 2 g of ammonia penetrates to the ROS. In this case the ROS hardware seems to be able to clean the ROS to acceptable levels, and probability of maintaining crew safety and ISS operations after the catastrophic ammonia release is higher.

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