Guidelines for the Assessment of Chemicals and Materials for Impacts to Environmental Control and Life Support Systems and Habitable Volumes of Crewed Spacecraft

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Environmental Control and Life Support Systems
Crew and Thermal Systems Division
Engineering Directorate

September 2015 Baseline

Cleared for Internal NASA Release

National Aeronautics and Space Administration
Lyndon B. Johnson Space Center
Houston, Texas

Guidelines for the Assessment of Chemicals and Materials for Impacts to Environmental Control and Life Support Systems and Habitable Volumes of Crewed Spacecraft

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1.0 INTRODUCTION

This document describes the procedural approach and acceptability guidelines used by NASA to perform assessments of Environmental Control and Life Support (ECLS) system hardware and process compatibility and the resulting impact on the cabin environment presented by chemicals and/or materials that may be vented and/or released into a crewed cabin environment. ECLS Systems Engineering is responsible for conducting the ECLS System Compatibility and Cabin Environmental Impact Assessments to provide the information necessary for assigning hardware and environment impact rating for all chemicals and materials that are used or transported in the habitable areas of NASA spacecraft, international vehicles (crewed and uncrewed), and commercial vehicles (crewed and uncrewed) that dock with crewed NASA spacecraft and habitats.

The approach for conducting ECLS system hardware and process compatibility, and cabin environmental assessments focuses on identifying and quantifying the relevant impacts associated with an inadvertent release of a chemical or material into a spacecraft cabin atmosphere. The results of the ECLS system hardware and process compatibility assessment combined with a cabin environmental impact assessment complement toxicological, radiological, microbiological, and flammability hazard assessments. Together, these assessments for the basis for mission-specific Hazardous Materials Summary Tables (HMST). These complementary assessments, considered together, serve to define that range of hazards that may be associated with a specific chemical or material when released into a crewed cabin environment. The assessment of toxicological, radiological, biological, and flammability hazards are beyond the scope of the guidelines and procedures documented herein. Subject matter experts in ECLS system engineering, toxicology, radiation exposure, microbiology, and fire prevention conduct these complementary hazard assessments that are included in an overall safety assessment package.

1.1 PURPOSE OF ECLSS IMPACT ASSESSMENTS

Safety is the highest priority to NASA, and as such, minimizing adverse effects on crew health in spacecraft and assuring mission success is a major NASA objective for crewed space exploration missions. Contamination of the cabin environment of crewed spacecraft and loss of ECLS system functionality can have an adverse effect on crew health, safety, and mission success. In supporting NASA’s safety and mission success objectives, ECLS System Engineering assumes responsibility for assessing the potential impacts on ECLS system hardware and processes as well as the vehicle cabin environment from all in-flight chemicals and/or materials that may be released into the habitable environment either by design or inadvertently. Chemicals and materials include all experiment and technology demonstration payload chemicals under the review auspices of the NASA Payload Safety Review Panel (PSRP) for use or transport in the pressurized volume of visiting vehicles operated by NASA, international space agencies, and domestic and international commercial space transportation suppliers to a vehicle operated by NASA or hosting NASA astronauts as well as other potentially toxic materials not reviewed by the PSRP. The latter include but are not limited to system and utility chemicals and those in government furnished equipment (GFE), risk mitigation experiments (RMEs), Development Test Objectives (DTOs), technology demonstrations, etc. Also applicable are chemicals and materials contained in vehicle systems that are operated by NASA, international space agencies, and domestic and international commercial space transportation suppliers and interface with NASA vehicles. Understanding the impacts chemicals and materials may have on the ECLS system and the cabin environment early in the payload or system design stage can help minimize or even prevent costly redesigns.

The assigned ECLS system compatibility and cabin environmental impact ratings can be used by payload and system developers as criteria in the design of flight hardware to assure adequate containment or by operations to develop flight rules and/or procedures to ensure ECLS system protection and minimal contamination of the habitable volume in the event of an inadvertent release. For experiments and other payloads flying in the pressurized volume of vehicles that dock to and/or resupply an established, crewed NASA vehicle or habitat, it is the responsibility of the PSRP to certify that the design of equipment provides adequate hazard controls for the chemicals and/or materials it contains. For vehicle systems flying in the pressurized volume of vehicles that dock to and/or resupply an established, crewed vehicle or habitat, it is the responsibility of the SRP to certify that the design of the equipment provides adequate hazard controls for the chemicals and/or materials the system contains and/or uses. The protocols in the HMST will help the crewmembers and flight operations to respond appropriately in the event of an inadvertent release of materials.

A chemical and/or material may be a solid, liquid, or gas. They may be pure chemicals, solutions, mixtures, solid or liquid aerosols, and/or metallic alloys. Chemicals and/or materials may originate from other sources within the payload and/or system, e.g., blood components, normal human or animal cells, human or animal cancer cells, microorganisms, plants, small animals, etc. During processing, test chemicals and/or materials may undergo changes in phase (e.g. solid or liquid to vapor or fume), undergo chemical reactions to produce new chemicals and/or materials (e.g. combustion), or undergo changes in concentration (e.g. dilution). The resulting chemicals and/or materials from these changes must also be assessed. Chemicals and/or materials can be classified as organic, inorganic, polymeric, biological, or radioactive and may possess acidic, basic, neutral, oxidizing/non-oxidizing, hypertonic/hypotonic, and hygroscopic properties or characteristics.

1.2 COMPILATION AND DISTRIBUTION OF ECLSS IMPACT ASSESSMENTS

The assessment process, derived from Reference 1 and shown schematically in Appendix A, begins with payload investigators, vehicle system designers, managers, or coordinators (collectively termed as payload or system design customers) submitting information and relevant data to the NASA Toxicology Group on payload/system chemicals and/or materials as described in JSC 27472, *Requirements for Submission of Test Sample Material Data for Payload Safety Evaluation* or its subsequent revisions. The relevant data, together with the assigned toxic hazard levels, are entered into a computerized database from which is generated an HMST. Payload chemicals undergo several verifications per JSC 26895, *Guidelines for Assessing the Toxic Hazard of Spacecraft Chemicals and Test Materials*. Payload/system design customers requesting an ECLS System Impact Assessment will be provided a report. A copy of this report will also be provided to the NASA Toxicology Group to update the HMST database, but it is the responsibility of the payload or system design customers to ensure NASA Toxicology is informed of the ECLSS Impact Assessment. Depending on the complexity of the assessment, this report may be as simple as an email or be in the form of a detailed report with a transmittal memorandum. The level of reporting detail required is determined by agreement between the performing ECLS system engineering organization and the payload/system design customer.

2.0 ECLSS AND CABIN ENVIRONMENT IMPACT RATING DEFINITIONS

Definitions of the ECLS System Hardware Impact and Cabin Environment Impact ratings are listed in Appendix B. The ECLS System Hardware Impacts Ratings are listed in terms of impacts to system resources, consumables, and the rated service life of the system and/or critical components of the system. The general timeframe to manifest orbital replacement units (ORUs) and/or other consumables is also listed for each impact level. The ECLS System Hardware Impact levels range from *E0* for no impacts to ECLS systems to *E6* for catastrophic impacts to the operability of ECLS systems. The Cabin Environment Impact ratings are listed in terms of the ability of ECLS systems to recover the cabin atmosphere to marginally acceptable levels. As such, the Cabin Environmental Impact assessment considers a chemical's and/or material's persistence in the cabin environment. The marginally acceptable rating is defined as below any mask donning requirement, typically the short-term U.S. spacecraft maximum allowable concentration (SMACs). The Cabin Environment Impact ratings range from *A* for 0-2 hours required to recover to E for greater than 168 hours (1 week) to recover or if ECLS systems are unable to remove the contaminant from the cabin atmosphere and it remains in the environment.

3.0 IDENTIFYING CHEMICALS IN PAYLOAD/HARDWARE

ECLS System Engineering assesses the potential impacts of chemicals and/or materials used or contained in vehicle systems and in in-flight payload experiments, equipment, and hardware (e.g. GFE, crew escape equipment, etc.) on ECLS system hardware and the cabin environment of crewed spacecraft. Usually, the information on chemicals/test materials is provided by mission managers, payload integration managers, or investigators. Payload and system design customers and sponsors of new GFE items generally are required to submit to the NASA Toxicology Group information on chemical identities, composition, physical states, concentrations, amount, test conditions and other relevant information, as specified in JSC 27472, *Requirements for Submission of Test Sample Material Data for Payload Safety Evaluation*, as part of their safety data packages prepared for payload safety reviews.

Subsequently, mission managers, payload integration managers, investigators, system design customers, or sponsors of new GFE items may request ECLS System Engineering to perform an ECLS system hardware and cabin environment impact assessment. It is the responsibility of the payload or system design customer to provide the latest safety data package (SDP) and any other information regarding the chemical(s) in the payload/hardware. This information includes material safety data sheets (MSDS), purity, and amounts. If the payload/hardware will be using previously flown hardware, then details (for example, the latest SDP) of the previously flown hardware should be provided by the payload customer. It is also the responsibility of the payload or system design customer to provide a credible release scenario and the amount of chemical(s) that can be released in this scenario. This information is critical to the ECLS system and cabin environmental impact analysis. If a credible release amount is not provided by the payload customer, then the release of the entire amount of the chemical(s) will be used in the assessment. If this amount is different from the amount used by NASA Toxicology in their assessment, then the amount used by NASA Toxicology will be used in the ECLS system hardware and cabin environment impact assessment.

Chemical and/or material data will be acquired from the payload/system design customer, material safety data sheets (MSDS), manufacturer's and supplier's literature, and the chemical literature. Physical property data will be acquired from published literature. In the absence of published literature, physical properties may be estimated using documented techniques. Recommended sources are provided by Appendix C.

4.0 GENERAL GUIDELINES BY WHICH ECLSS HARDWARE IMPACTS AND CABIN ENVRIONMENT IMPACTS ARE ASSESSED.

4.1 REQUIREMENTS

Because the specification of the active trace contaminant control equipment for a spacecraft precedes those data necessary to fully validate its design, standard design practice dictates a conservative approach whereby the active contamination control system performs its function unassisted by any other systems or processes in the cabin.[2] As such, overboard atmospheric leakage and assists provided by other air processing systems such as CO_2 removal and humidity control equipment are not considered during the design and validation of the active trace contaminant control equipment.

Ideally, all new potential contaminant loads are assessed in the same manner in order to maintain consistency. However, ECLS systems, in particular trace contaminant control systems, could vary from one vehicle to another depending on the mission. As a result, requirements levied on vehicle systems will vary from one vehicle to another depending on the mission. Despite this variation, the cabin air quality design approach should remain relatively consistent irrespective of vehicle and mission. This approach centers around three basic elements – air quality standards, active control, and passive control.[3] Generally, crewed NASA vehicles and those designed to dock to crewed NASA vehicles employ the acceptable-risk levels set by the SMACs as air quality standards. Interface conditions with the primary vehicle that govern the conditions at docking and subsequent hatch opening for a visiting vehicle are derived from the SMACs as well as consider the ECLS system compatibility limits of the primary vehicle. Interface documents and flight rules governing vehicle air quality interfaces and hatch opening criteria are considered as part of the ECLS compatibility and cabin environmental impact assessments. Appendix D provides an example of interface conditions for vehicles docking to the ISS.

In general, crewed space exploration vehicles must control individual trace chemical contaminants in the cabin atmosphere below their respective Spacecraft Maximum Allowable Concentrations (SMACs) as defined by the latest revision of JSC 20584. Crewed space vehicle programs and projects adopt the SMACs as the governing air quality standard to design the passive and active trace contaminant control methods. The active trace contaminant control equipment is designed to accommodate the vehicle’s basic equipment off gassing load plus the metabolic load from a specified crew size complement to comply with the SMAC limits. Crewed space vehicle trace contaminant control equipment design performance specifications and relevant performance documentation serve as the basis for assessing the basic ECLS system’s action on a contamination load resulting from a chemical and/or material release into the cabin environment.

The incidental removal of trace contaminants by other ECLS system equipment is not considered for the active trace contaminant control equipment design; however, incidental removal by other ECLS system equipment and processes is used to evaluate the fate of chemical contaminants as part of the ECLS system compatibility and cabin environmental impact assessment. Performance requirements for the active trace contaminant control equipment aboard a crewed spacecraft will have been verified by previous engineering analyses and functional tests. Documentation from these analyses and tests serve as the performance basis for the space vehicle’s active contamination control system.

Further guidance may be provided by a space vehicle program's Medical Operation's Requirements Document (MORD). Using the ISS as an example, SSP 50260, *Medical Operations Requirements Document* (MORD), outlines an operational philosophy in which Russian limiting permissible concentrations (LPCs) are defined as "zero risk" concentrations and NASA SMACs are defined as "acceptable risk" concentrations. According to various Multilateral Medical Operations Panel (MMOP) air quality group bilateral agreements, the acceptable risk concentrations must not be exceeded during normal *ISS* operations. The zero risk concentrations are the goal for active air quality control during normal operations. Short duration concentration transients between the limits are permitted and expected.

Within the context of requirements, an additional loading of a chemical compound and/or material not contained in the design performance specification for a space vehicle's trace contaminant control equipment constitutes a new, specific verification case. As such, this verification must assume that only the active contamination control systems on board the crewed space vehicle removes the added contamination load. This maintains consistency with the equipment's certification. It is informative to expand the assessment, however, to address the fate of the contamination to ensure that the impact upon all ECLS system processes—both atmospheric and water processing—are addressed.

Cabin air quality interface requirements, flight rule guidelines, emergency response guidelines to toxic atmosphere events, guidelines pertaining to hatch opening and cabin atmosphere exchange between a primary crewed space vehicle and a visiting vehicle, and other guidelines are considered as appropriate for the specific space vehicle program.

4.2 APPROACH

The approach to determine the ECLS System Hardware Compatibility and Cabin Environment Impact ratings are essentially the same for all chemicals and/or materials regardless of their naturally occurring state. Solids and liquids can affect the service life of particulate air filters or require more frequent housekeeping maintenance. Also, highly volatile solids and liquids can affect air revitalization and water processing systems in the same manner as gases. Any reaction products generated by the payload or system hardware will be considered and may have an effect on the ECLS system hardware and cabin environment impact ratings assigned. Reaction products generated from the exposure of the released chemical(s) and/or material(s) as well as impurities contained in the released chemical(s) and/or material(s) to high temperature processes contained in space vehicle ECLS systems or due to the reactivity of the released chemical(s) under cabin environmental conditions (e.g. decomposition, reaction with humidity, and other) will be considered and may have an effect on the ECLS System Hardware and Cabin Environment impact levels assigned. The presence of impurities in the chemical(s) and/or material(s) will be considered and may have an effect on the ECLS System Hardware and Cabin Environment impact ratings assigned.

4.3 CASES CONSIDERED

Cases considered are to be based on credible release scenarios provided by the payload/system design customer. If this is not provided, release of the entire amount of the chemical is assumed and will be noted in the assessment. Other cases considered in the assessment will be noted in the report. Additional guidance relating to assessing chemical releases can be found in Reference 4.

It will be assumed that for the entire duration the chemical(s) and/or material(s) is on board the crewed space vehicle, that the vehicle program's nominal crew size complement will be present. Cases to evaluate sensitivities associated with varying crew size complements may be considered based on agreement between the ECLS System Engineering organization and the payload/system design customer. The number of crew members may affect the Cabin Environment Impact rating for water-soluble chemicals due to changes in the latent load of the cabin atmosphere. In the event of a release of the chemical, emergency strategy and procedures require visiting crew to evacuate to their vehicle.

4.4 VEHICLE CONFIGURATION

Vehicle configuration is critical to understanding the impacts contaminants may have on ECLS systems and the cabin environment. Vehicle configuration defines the habitable volume and the atmosphere scrubbing assets available. Space vehicle design cabin, ECLS system, and ventilation system design documentation will serve as the basis for establishing the cabin free volume, cabin environmental conditions, cabin ventilation architecture and flow rates, and contaminant removal device flow rates. The ECLS System Engineering organization will work with the appropriate space vehicle program office to acquire the necessary documentation to establish the proper vehicle configuration.

4.5 ANALYZING THE HAZARD OF CHEMICAL MIXTURES

The ECLS system hardware and cabin environment impact of a mixture of chemicals is set by the chemical determined to have the greatest ECLS system hardware and cabin environment impact.

4.6 ASSESSING CHEMICALS THAT UNDERGO PHASE OR COMPOSITION CHANGES DURING PROCESSING OR CONCENTRATION CHANGES AFTER MIXING

If chemicals or mixtures pose different impacts to ECLS system hardware and/or the cabin environment before, during, or after these chemicals are processed, all of these stages will be assessed. If a liquid is to be mixed with another liquid of a different impact level, then the resultant mixture also is assessed.

4.7 CABIN MASS BALANCE

Assessing the capability of the atmospheric quality control systems aboard crewed space vehicles to effectively control chemical releases into the cabin atmosphere as a result of an inadvertent release to below specified limits requires two stages. The first assumes the entire primary vehicle cabin is a well-mixed volume and that the effective removal term, $\Sigma\eta v$, remains constant with time. This makes the solution of the basic mass balance equation, shown by Equation 1, fairly simple. The solved form of the equation is shown by Equation 2. Reference 5 documents the derivation of Equations 1 through 5. In Equations 1 and 2, m is the contaminant mass at time, t; m_o is the contaminant mass at time equal to zero; V is cabin volume; $\Sigma\eta v$ is the contaminant removal capacity; g is the contaminant generation rate; and t is time.

$$\frac{dm}{dt} = g - \left(\frac{\sum \eta v}{V}\right) m \tag{1}$$

$$m = m_o e^{-\left(\sum \eta v/V\right)t} + \left(gV/\sum \eta v\right)\left[1 - e^{-\left(\sum \eta v/V\right)t}\right] \tag{2}$$

In the event a contaminant release is large, the removal rate is assumed to be much greater than the contaminant generation rate and Equation 2 can be simplified to Equation 4.

$$C = C_o e^{-\eta v t / V} \tag{3}$$

Solving Equation 3 for time (t) can estimate the time required for cabin contaminant removal yields Equation 4. If more than one scrubbing asset is available, the total effective removal rate, ηv, will be the sum of the effective removal rates for each asset. Performance data documenting capability of each removal asset serve as the basis for the total effective removal rate.

$$t = -\left(V / \sum \eta v \right) \ln \left(C / C_o \right) \tag{4}$$

Approximate removal times can be determined using an average removal efficiency of 50% for adsorption-based removal devices.

The second stage assumes that in the case of an inadvertent release, conditions approach those of a steady state. At steady state conditions, Equation 2 reduces to a very simple form involving only the generation rate, cabin volume, and effective removal terms as shown by Equation 5.

$$m = gV / \sum \eta v \tag{5}$$

Equations 1 through 5 are suited for a space vehicle consisting of a single module or for a multi-volume vehicle with very efficient ventilation. Even with effective ventilation, the propagation of contamination between two adjacent space vehicle modules may need to be assessed. In the case of a multi-module vehicle or two docked vehicles that exchange cabin atmosphere through forced ventilation leading to contamination propagation between the two volumes, a more rigorous mass balance approach is necessary. This more rigorous mass balance between two adjacent spacecraft volumes helps to examine the duration of a transient event between the volumes. This more rigorous mass balance requires the simultaneous solution of the mass balance equations for each individual volume. The mass balance equations for the two adjacent volumes are provided by Equations 6 and 7, respectively.[6] These equations define the change in contaminant mass as a function of time.

$$\frac{dm_A}{dt} = \frac{\dot{v}_B}{V_B} m_B - \frac{\dot{v}_A}{V_A} m_A - \frac{\sum \eta v}{V_A} m_A + g_A \tag{6}$$

$$\frac{dm_B}{dt} = \frac{\dot{v}_A}{V_A} m_A - \frac{\dot{v}_B}{V_B} m_B - \frac{\sum \eta v}{V_B} m_B + g_B \tag{7}$$

In Equations 6 and 7, m_A is the total mass of contaminant in volume A, m_B is the total mass of the contaminant in volume B, V_A is the free volume of volume A, V_B is the free volume of volume B, $\dot{v}_A$ is the ventilation flow from the volume A to volume B, $\dot{v}_B$ is the ventilation flow from volume B to volume A, $\Sigma\eta v$ is the removal capacity in the respective volume, g_A is the generation rate in volume A, and g_B is the generation rate in volume B.

Simultaneous solution of Equations 6 and 7 provide an equation for each volume in the form of Equation 8. In Equation 8, *m* is the total mass of contaminant in the reference cabin volume; α, β, and γ are constants calculated from the segment cabin free volume, ventilation flow, removal capacity, and contaminant generation rate; and x_2 and x_3 are 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.

$$m = \alpha + \beta e^{x_x t} + \gamma e^{x_3 t} \tag{8}$$

If the entire cabin volume is assumed to be well mixed, or each volume is isolated, the total cabin mass balance equation can be defined more simply as Equation 2.

Beyond this level of evaluation which is conservative due to the assumption that the cabin volumes are instantaneously well mixed, a closer approximation of the contamination dispersion dynamics can be accomplished using computational fluid dynamics (CFD) models of the space vehicle cabin(s) and/or multi-vehicle cabin and ventilation configuration. The complexity of the dispersion cabin concentration dynamic analysis will be determined by the ECLS System Engineering organization and the payload/system design customer.

4.8 LIQUID EVAPORATION RATE ESTIMATION

Estimating evaporation rate from a gross leak of fluid is accomplished using calculation techniques documented in the literature and employed by the U.S. Environmental Protection Agency (EPA) for assessing environmental impacts of chemical spills. The equation used for this calculation requires information on air velocity, vapor pressure, molecular weight, and leaked surface area. Equation 1 estimates the evaporation rate, *QR*, in lb/minute.[7] In Equation 9, *M* is molecular weight in g/mole, *A* is the leaked pool surface area in ft^2, T is absolute temperature in Kelvin, P_V is vapor pressure in mm Hg, and *u* is air velocity in m/s.

$$QR = \frac{0.284 u^{0.78} M^{2/3} A P_V}{82.05 T} \tag{9}$$

Equation 1 is used to estimate the evaporation rate from a leaked volume of a fluid. Evaporation from binary liquid mixtures is evaluated by applying Eq. 1 to the calculation method described by Blanchard and Hadlock.[8] It should be noted that Equation 1 does not take into account effects associated with evaporative cooling such as more rigorous methods employed in the EPA's Area Locations of Hazardous Atmosphere (ALOHA) software. The results from Equation 1, however, are conservative relative to results obtained when using the more complex ALOHA software. Reference 4 indicates that multiplying the result from Equation 1 by 0.63 accounts for the conservatism associated with this approach relative to that employed by the EPA's ALOHA software.

4.9 HUMIDITY CONDENSATE LOADING ESTIMATION

In addition to removal by the active contamination control equipment, water soluble contaminants are also removed by absorption in humidity condensate. As noted earlier, the assist provided to the active contamination control equipment on board spacecraft the employ a condensing heat exchanger for humidity control is considered only to address potential impacts to water processing systems that might be part of a space exploration vehicle's ECLS system, such as found on the International Space Station or planned for future space vehicles and/or habitats.

This removal method can be quite effective for water-soluble chemicals such as volatile alcohols, aldehydes, short-chain esters and ketones. It is assumed that such contaminants are present at relatively low concentrations and, as such, can be considered to be infinitely dilute. Under this condition, Henry's Law, Equation 10, can be applied to relate the partial pressure in air, p_i, to the liquid mole fraction, x_i, and Henry's constant, H.

$$p_i = Hx_i \tag{10}$$

By applying Henry's Law to the humidity condensate mass balance, the liquid and vapor phase mole fractions of a contaminant as a function of the gas and liquid flow rates can be obtained.[9-10]

$$x = y \Big/ \left(C/A + H/P \right) \tag{11}$$

In Equation 11, x and y are the liquid and vapor phase molar fractions, respectively, C and A are the condensate and gaseous molar flow rates, respectively, H is Henry's Law Constant for the contaminant, and P is the total pressure. Other assumptions involved in Equation 11 include: (1) the gaseous contaminant concentration is uniform, (2) gas phase and liquid phase mass transfer is negligible, (3) mass transfer across the gas-liquid interface is fast, and (4) concurrent absorption occurs after condensation. To account for liquid phase dissociation and reaction, temperature effects, and heat exchanger geometry that contribute to deviation from strict Henry's Law behavior, an adjustment factor, α, is introduced as shown by Equation 12.

$$x = y \Big/ \left(C/A + \alpha H/P \right) \tag{12}$$

The adjustment factor has been shown to account for chemical dissociation or reaction in the liquid phase and temperature effects in the condensing heat exchanger that contribute to deviation from strict Henry's Law behavior. Temperature effects are typically accounted for by multiplying the Henry's Law constant by the vapor pressure ratio for the condensing heat exchanger temperature to the vapor pressure at 20 °C.[11] Further, dividing the adjusted Henry's Law constant by 3 has been shown to account for bulk liquid surface area differences experienced between 1g and micro-g conditions.[12] Equation 12 is used to calculate the inlet and outlet concentration of a chemical and/or material for a condensing heat exchanger. Single pass removal efficiency is calculated using the inlet and outlet concentration.

4.10 ACTIVATED CARBON LOADING BY VOLATILE ORGANIC COMPOUNDS

Calculation of activated carbon loading is based upon the Polanyi adsorption potential theory.[13-14] The adsorption potential, as defined by Equation 1, is used to calculate the equilibrium activated carbon loading. In Equation 13, T is temperature in Kelvin, V_m is the liquid molar volume at the normal boiling point in cm^3/g mole, C_s is vapor pressure expressed in concentration units, mg/m^3, and C is the cabin concentration in mg/m^3.

$$A = (T/V_m)\log_{10}(C_s/C) \tag{13}$$

The potential factor is used in a Freundlich-type isotherm equation shown in its general form by Equation 14.

$$q = \alpha e^{-\beta A} \tag{14}$$

In Equation 14, the activated carbon loading, q, is in cm^3 liquid contaminant/g charcoal, and the pre-exponential factor, α, is 2.1 for soluble compounds and 1.41 for insoluble compounds at 50% relative humidity. The exponential factor, β, is 0.31.

The preceding factors are correlations for Barnabey Sutcliffe Type 3032 activated carbon used in the active trace contaminant control equipment aboard the International Space Station. These correlations can be used for estimating loading magnitude for other activated carbon products; however, it is highly recommended that correlations specific to a particulate activated carbon product be used when available.

Additional information on trace contaminant removal equipment performance and the fate of trace contaminants in spacecraft cabins that are useful guides is documented by References 15-17.

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APPENDIX A—ASSESSMENT PROCESS AND INFORMATION FLOW

Figure A-1. Chemical Assessment Process

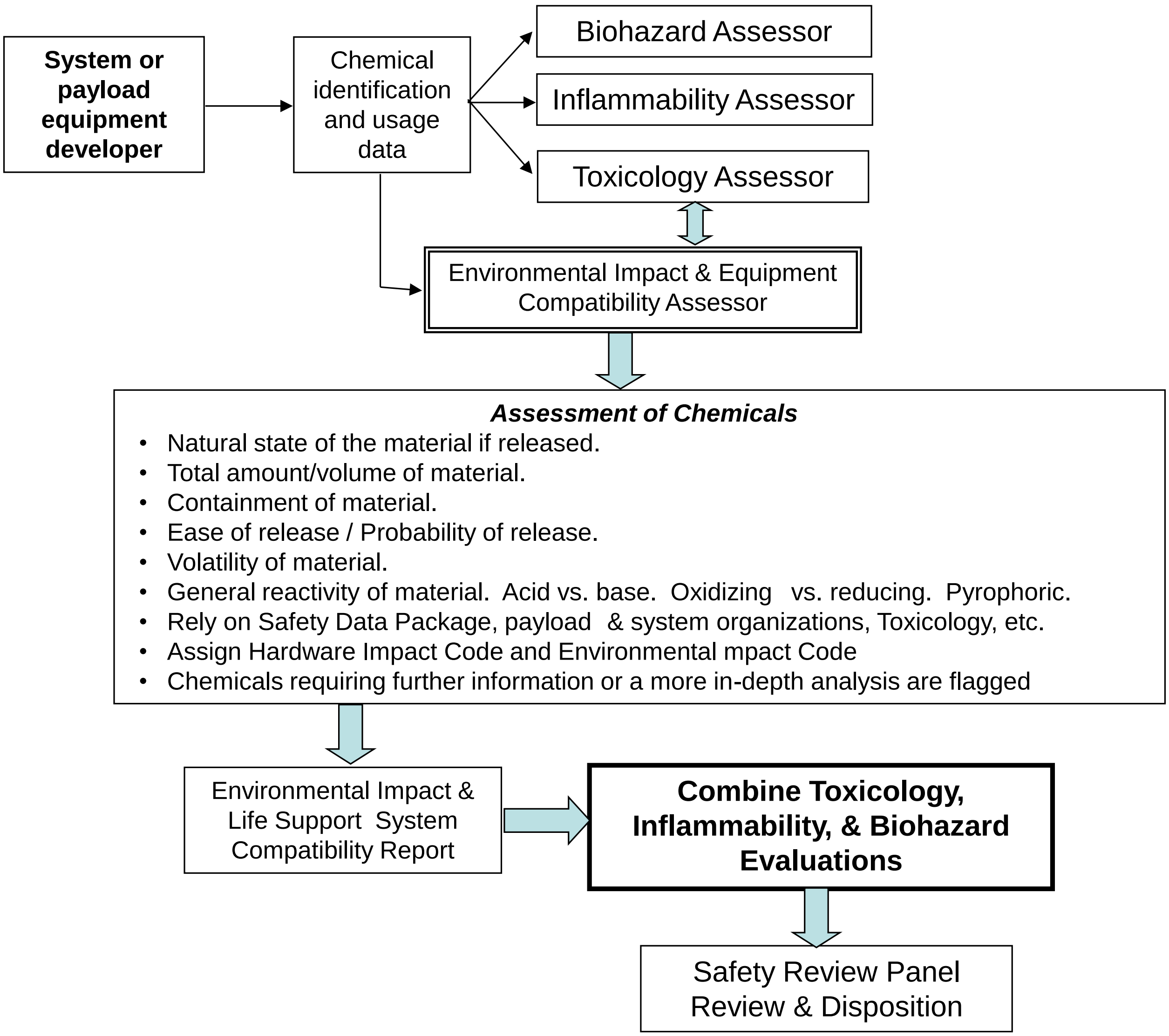
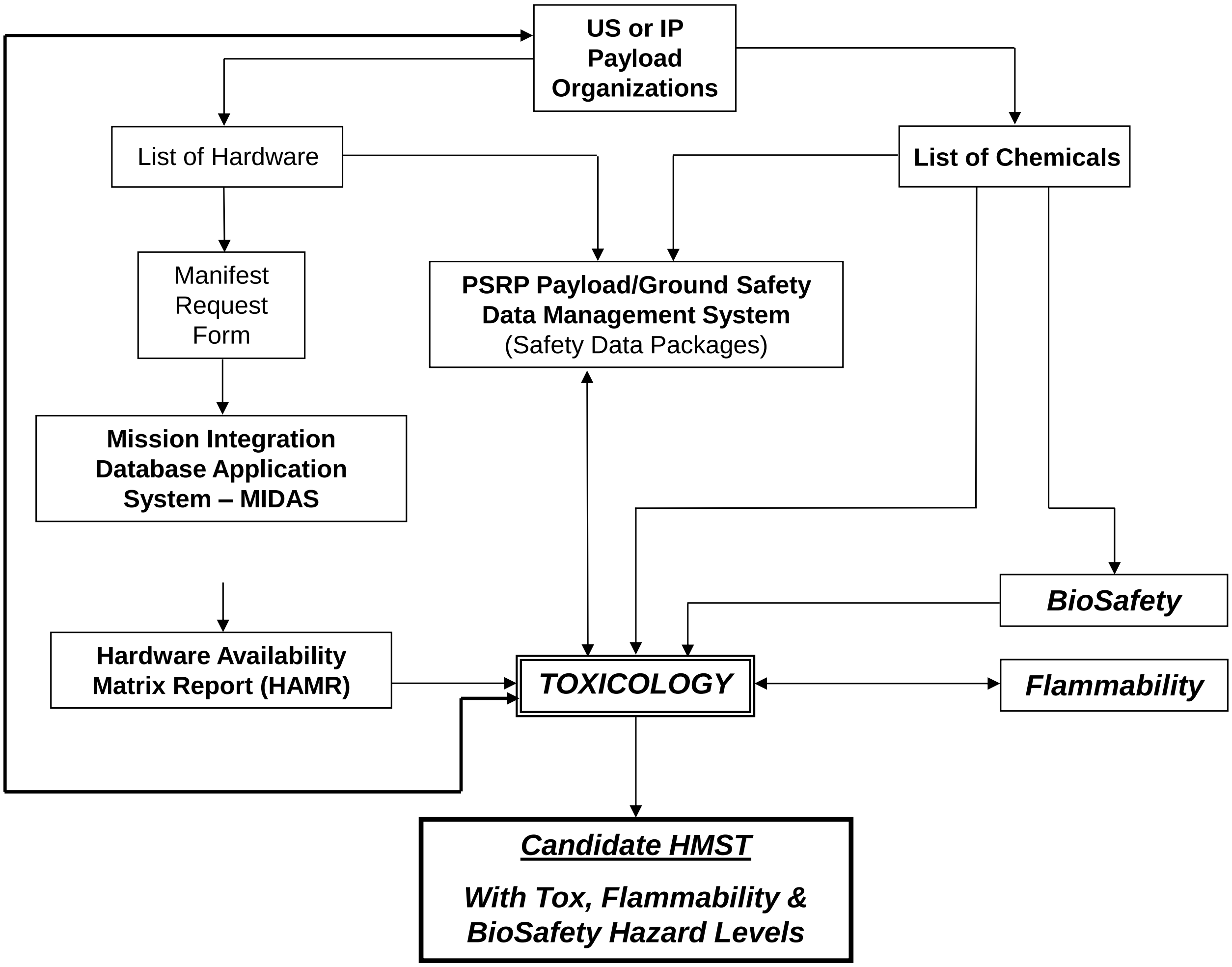


Figure A-2. Simplified Chemical and Material Information Flow



APPENDIX B—ECLS SYSTEM AND CABIN ENVIRONMENTAL IMPACT DEFINITIONS

ECLSS Hardware Impact Definitions

E0 – **No Impact** on ECLS Systems. The rated service life of system consumables are reduced on the order of <2% associated with the off-nominal event.

E1 – **Minor Impact** on the ECLS Systems resources/consumables. The rated service life of system consumables are reduced on the order of >2% and <10% associated with the off-nominal event. At least 50% of the ECLS System functional margin is retained.

E2 – **Moderate Impact 1** on the ECLS Systems resources/consumables. The rated service life of system consumables are reduced on the order of >10% and <25% associated with the off-nominal event. Functional margin is consumed but there is no ECLS functional capacity degradation.

E3 – **Moderate Impact 2** on the ECLS Systems resources/consumables. The rated service life of system consumables are reduced on the order of >25% and <50% associated with the off-nominal event. No functional margin is retained and early manifesting of replacement consumables may be necessary. ECLS functional capacity degradation is <25%.

E4 – **Critical Impact 1** on the ECLS Systems resources/consumables. The rated service life of system consumables are reduced on the order of >50% associated with the off-nominal event. Greater than 50% reduction of the rated service life of consumables may cause an expedited change-out, but would not require immediate change-out. Requires early manifesting of replacement consumables. No functional margin is retained and ECLS functional capacity degradation is >25% and <50%.

E5 – **Critical Impact 2** on the ECLS Systems resources/consumables. Requires immediate change-out of a system consumable or component(s) or some additional system cleaning/maintenance. Requires early/immediate manifesting of replacement consumables. This would result in the loss of crew life support capability without immediate system restorative maintenance. No functional margin is retained and ECLS functional capacity is degraded by >50%.

E6 – **Catastrophic Impact** to the operability of ECLS Systems. Causes permanent contamination of system components such that the system cannot recover operability by simple ORU or component(s) change-out or cleaning/maintenance. This would result in the loss of crew life support capability and loss of mission. No functional margin is retained and ECLS functional capacity is degraded by >75%.

Cabin Environmental Impact Level Definitions

(Ability of ECLSS to Recover Atmosphere)

A – Time for ECLS systems to recover Environment to marginally acceptable levels is 0-2 hours.

B – Time for ECLS systems to recover Environment to marginally acceptable levels is 2-24 hours.

C – Time for ECLS systems to recover Environment to marginally acceptable levels is 24-72 hours (1-3 days).

D – Time for ECLS systems to recover Environment to marginally acceptable levels is 72-168 hours (3 days - 1 week).

E – Time for ECLS systems to recover Environment to marginally acceptable levels is greater than 168 hours (1 week) **OR** ECLS system unable to remove substance and it persists in the cabin environment.

APPENDIX C—CHEMICAL INFORMATION SOURCES

Useful Chemical and Physical Property Sources

Poling, B. E., Prausnitz, J. M., and O'Connell, J. P., *The Properties of Gases and Liquids, 5th Edition,* McGraw-Hill, 2001.

Lewis, R. J., *Hawley's Condensed Chemical Dictionary, 15th Edition,* Wiley. *http://onlinelibrary.wiley.com/book/10.1002/9780470114735*

CRC Handbook of Chemistry and Physics, CRC Press.

Estimation Program Interface (EPI) Suite, U.S. Environmental Protection Agency, *http://www.epa.gov/opptintr/exposure/pubs/episuite.htm*

ChemSpider, *http://www.chemspider.com/*

Korea Thermophysical Properties Data Bank (KDB), *http://www.cheric.org/kdb/kdb/hcprop/cmpsrch.php*

NIST Chemistry WebBook, *http://webbook.nist.gov/chemistry/*

ChEresources.com, *http://www.cheresources.com/content/articles/physical-properties/physical-properties-on-the-internet*

Chemeo, *http://chemeo.com/*

APPENDIX D—EXAMPLES OF CHEMICAL CONCENTRATION THRESHOLDS FOR DOCKED VEHICLES

Table D-1. Polar Compound Concentration in Visiting Vehicle Cabin Atmosphere at Hatch Opening with ISS

COMPOUND	CONCENTRATION	
	(mg/m^3)	(ppm)
Methanol	9	7
Ethanol	50	27
Isopropanol	150	60
n-propanol	1.5	0.6
n-butanol	15	5
Acetone	50	20
Ethylene glycol	0.1	0.04
Propylene glycol	46	15
Glycerol	0.1	0.03

Table D-2. Maximum VOC Concentration in Visiting Vehicle Cabin Atmosphere at Hatch Opening with ISS

(Visiting vehicle cabin volume basis is Orion)

COMPOUND	TOTAL RELEASED MASS (grams)	ISS ECLSS CONCENTRATION THRESHOLD (mg/m^3)	AFFECTED ECLSS HARDWARE	NOTES
Ammonia and volatile amines	170 75% of TCCS CBA capacity	3.5	TCCS charcoal bed assembly (CBA) service life impact.	Can form NO_x in contact with hot surfaces so is also SFOG operational constraint. Release rate >2.6 gram/day exceeds TCCS scrubbing rate.
Halocarbons including Bromotrifluoromethane (Halon 1301), Hydrofluorocarbons (HFCs), Perfluorocarbons (HFE , Fluorinert , and Galden fluids)	50 75% of TCCS SBA capacity as dichloromethane basis	2	TCCS sorbent bed assembly (SBA) service life impact.	May form acid gases in contact with hot surfaces so is a solid fuel oxygen generator (SFOG) operational constraint. Concentration >2 mg/m^3 concentration entering TCCS COA results in >40% loss of methane oxidation performance. Performance loss is partially recoverable with estimated 10% permanent oxidation efficiency loss.
Sulfur compounds (excluding SF_6)	2 hydrogen sulfide basis	1	Irreversibly poisons TCCS catalytic oxidation assembly (COA) catalyst.	Forms SO_2 upon oxidation. Concentration of 1.4 mg/m^3 concentration entering the COA results in irreversible 40% loss of methane oxidation performance. SF_6 has been shown to not react in the COA.
Thionyl chloride	5 75% of 2 $LiSOCl_2$ ½ AA batteries basis	6	TCCS SBA service life impact and irreversible TCCS COA catalyst poison.	Decomposes to SO_2 and HCl on contact with humidity in the atmosphere. Single ½ AA $LiSOCl_2$ battery leak may result in 70% loss of TCCS COA activity.
Organosilicones (silicone-based liquids and grease):	316 75% of TCCS CBA capacity as trimethylsilanol basis	4	Irreversible TCCS COA catalyst masking and Russian BMP ZPL-1M regenerable carbon bed fouling.	Organosilicone compounds are one of the higher concentration contaminants in the ISS cabin air. Could also have some deleterious effect on heat exchanger coating performance and water processor.
Polar volatile organic compounds: methanol ethanol	0.07 2.5	0.1 4	Water processor assembly (WPA) performance and logistics impacts.	Excessive humidity condensate loading leads to overall process inefficiencies and expendable resource consumption.

COMPOUND	TOTAL RELEASED MASS (grams)	ISS ECLSS CONCENTRATION THRESHOLD (mg/m^3)	AFFECTED ECLSS HARDWARE	NOTES
isopropanol n-propanol n-butanol acetone ethylene glycol propylene glycol glycerol	2.5 0.14 1 2.5 0.007 3 0.02	4 0.2 1.4 4 0.01 5 0.03		Logistics resupply and recurring operating cost impacts.
Other water-soluble volatile organic compounds: Dimethyl sulfone Chloroethanol Iodoacetamide Chloroacetone Dichloroacetone Methylene chloride Methylene bromide Bromacetone Dimethyl sulfoxide 2,2-thiodiethanol Chloroacetaldehyde Tribromoethanol Chloroacetonitrile Methyl iodide Ethyl bromide 1,3-dichloro-2-propanol Dimethyl thiourea Ethylene bromohydrin; Chloroacetamide Thiourea Methanethiol Methyl bromide Ethanethiol 2-Mercaptoethanol Thioformamide Thioacetamide Dichloroacetonitrile Ethylene thiourea Methylene iodide	<0.7	<1	Water processor assembly (WPA) volatile removal assembly (VRA) catalyst poisoning.	If present in significant quantities these compounds may load humidity condensate excessively. At high humidity condensate loadings (e.g., due to a spill), these compounds could break through the ISS WPA multi-filtration beds and reach the oxidation reactor. The reaction rate in the reactor is so slow that they act as a poison by occupying catalyst sites and preventing the oxidation of other volatile organic compounds.

COMPOUND	**TOTAL RELEASED MASS (grams)**	**ISS ECLSS CONCENTRATION THRESHOLD (mg/m^3)**	**AFFECTED ECLSS HARDWARE**	**NOTES**
Bromoacetamide				

Note 1: See Table D-1.
Note 2: SMAC value for compound driving threshold limit.