54th International Conference on Environmental Systems
13-17 July 2025, Prague, Czech Republic

ICES-2025-450

Spacecraft Water Impurity Monitor (SWIM), a System for Water Quality Analysis on Exploration Missions Beyond LEO

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Exploration missions beyond low-earth-orbit (LEO) will require advanced instrumentation to monitor water quality. Traveling beyond LEO means the transfer of water samples to an Earth-based laboratory for detailed analysis is not possible. Detailed analysis of water composition during exploration is still necessary, because having the capability to determine the specific organic chemical causing a change in total organic carbon (TOC) or the specific metal or ionic species causing a change in conductivity has the potential to steer the crew health and system management decisions differently. On a new vehicle such as a lunar or Mars surface habitat or a Mars transit vehicle, the occasion of finding "new" impurities not seen on ISS should be expected. The key is to identify the impurity so the correct action can be taken. On ISS we can measure TOC, conductivity, and other physical properties but do not have the capability for detailed analysis using vehicle instrumentation. This is acceptable because ISS can send samples down to Earth for further analysis in a timely manner. For exploration, the inability to send samples to Earth is why SWIM is a necessary new technology suite. SWIM is the answer to detailed water quality analysis when sample down mass is not available. SWIM is a system comprising organic and inorganic modules. For organic chemicals, a gas chromatograph mass spectrometer (GCMS) detects and identifies organic impurities. For inorganic species, a capillary electrophoresis capacitively coupled contactless conductivity detection (CE-C4D) system as well as ion specific electrodes detect and identify metal ions and other inorganic salts / acids. The SWIM technology demonstration project is currently working to define requirements for an ISS technology demonstration of the organic and inorganic subsystems, while continuing to conduct technology feasibility and technology maturation efforts prior to beginning detailed system design for the flight instrument.

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Acronyms and Nomenclature

C&DH = command and data handling
CE = capillary electrophoresis
CE-C4D = capillary electrophoresis capacitively coupled contactless conductivity detection
COTS = commercial off the shelf
DMSD = dimethylsilanediol
EMU = extravehicular mobility unit
EPA = Environmental Protection Agency
EVA = extravehicular activity
FID = flame ionization detector
GC = gas chromatography
GCMS = gas chromatography mass spectrometry
ISE = ion selective electrode
ISS = International Space Station
IWM = inorganic water module
JPL = Jet Propulsion Laboratory
JSC = Johnson Space Center
LC = liquid chromatography
LEO = Low Earth Orbit
MS = mass spectrometer
MTH = Mars Transit Hab
NASA = National Aeronautics and Space Administration
OWM = organic water module
SRR = system requirements review
SWEG = Spacecraft Water Exposure Guideline
SWIM = Spacecraft Water Impurity Monitor
TEC = Toxicology and Environmental Chemistry
TIC = total inorganic carbon
TOC = total organic carbon
TOCA = Total Organic Carbon Analyzer
WRS = Water Recovery System

I. Introduction

WATER quality monitoring for crewed missions is of critical importance.[1] On the International Space Station (ISS) water quality is monitored on the vehicle using many sensors, including conductivity sensors and the Total Organic Carbon Analyzer (TOCA). Samples are down-massed from the ISS to the NASA Johnson Space Center (JSC) Toxicology and Environmental Chemistry (TEC) lab for detailed compositional analysis on a regular basis, because detailed compositional information about the water cannot be determined on orbit. This program of on-orbit monitoring plus downmass has been an effective and sufficient monitoring program. The TEC lab publishes water quality reports which are available publicly from NASA.[2]

A wealth of information has been learned about the performance of the water recovery system (WRS) of ISS over its operational lifetime.[3] In short, the water is always very clean, and system managers are able to use trending data from TOCA and other sensors to help prescribe maintenance intervals for WRS components such as multifiltration beds. Sometimes the program of onboard monitoring, coupled with ground analysis, enabled discovery of a new source of organic carbon in the water. Rising total organic carbon (TOC) levels were correlated with a known source, which is important regardless of level of hazard caused by the chemical. This was the case in identifying dimethylsilanediol (DMSD)[4] as the source for an increased TOC during a period of upward trending TOC values.

While much focus is placed on the safety and potability of the water consumed by the crew, clean water is necessary for hardware reasons such as WRS performance and extravehicular activity (EVA) hardware pre-processing or compatibility requirements. For example, the sublimator in the extravehicular mobility unit (EMU) has shown historical sensitivity to organic compounds,[5] and as suits get more advanced and systems are miniaturized, the potential for high sensitivity to impurities in spacecraft water increases.

Part of the requirements of the monitoring program is related to the timing of water quality measurements. A certain frequency of sampling is required for the monitoring program that is determined by system managers, flight doctors, and toxicology. This measurement cadence is well established for ISS, but for any new vehicles or surface habitats this is not yet determined. It can be projected that a monitoring frequency somewhere in the range of weekly at the most frequent up to as infrequently as quarterly would be reasonable. On ISS, TOC determinations are made on a weekly basis and samples are collected and transferred to the TEC lab on a roughly quarterly basis for detailed impurities analysis. Challenges for water monitoring on exploration missions arise when the vehicle is operating outside low earth orbit (LEO), for example the Mars Transit Hab (MTH) or a base on the surface of Mars. It is expected that a TOC analyzer will be included for the exploration environments, so the frequent monitoring of TOC can continue, but there will be no capability to downmass water samples to the TEC lab in a sufficiently fast timeframe for compositional analysis or to determine the identity of an unknown compound causing rising TOC or conductivity. Sensing of physical properties such as pH and conductivity will still be required for the water system, but again due to the inability to downmass samples, no capability for analyzing for metals and ions would be available from a TEC lab analysis. It takes months to transport water from an MTH or surface hab to the TEC lab, leading to an 8- to 12-month cadence for detailed water analysis, likely not frequent enough to support water monitoring program requirements.

The Spacecraft Water Impurity Monitor (SWIM) is a suite of technologies which enable on-orbit or in-habitat determination of more detailed water composition and impurity information. In order to analyze samples that are a complex mixture, a separation science based approach is applied. Separation science is described generally as a technique where a complex mixture is first separated into component parts so that the detector can analyze impurities one at a time. Separation science specifically includes technologies such as gas chromatography (GC), capillary electrophoresis (CE), and liquid chromatography (LC), among many others. Following separation, detection of each component of the mixture is achieved using a suitable detector. Many detectors are available for gas chromatography, such as thermal conductivity detection (TCD), flame ionization detector (FID), mass spectrometer (MS). Capillary electrophoresis detection methods include capacitively coupled contactless conductivity detection (C4D). The application of separation science is included in the operational trace contaminant monitor for ISS, the Air Quality Monitor. Separation science is not a novel technique, instead it is the *preferred* technique for mixture analysis.

SWIM will be capable of identifying organic contaminants in water samples using gas chromatography mass spectrometry (GCMS) detection, and will be capable of identifying inorganic contaminants using ion specific electrodes (ISE) and CE coupled with C4D detection (from here forward referred to as CE-C4D). In this paper we report on progress made on the SWIM project and preparations toward a flight technology demonstration. Updates on the required chemical target lists for organic and inorganic contaminants will be presented for the organic water module (OWM) and inorganic water module (IWM).

II. SWIM Architecture

The basic architecture of SWIM comprises sampling water and supplying that water to the inorganic and organic analysis modules for the analysis phase. For OWM, a GCMS determination of organic impurities is performed. For IWM, a CE-C4D determination of metals and ions is performed with specific ISEs used to monitor some species. Physical properties of the water such as conductivity can be monitored by the system either on a semi-continuous basis, or during routine sample analysis. The basic architecture for SWIM is shown in block diagram form in Figure 1. SWIM is a stand-alone water analysis system and will require power and data interfaces to the environment in which it operates, whether that be a vehicle or a habitat. Shown in the block diagram is a configuration that could sample both a water bus and also accept grab samples of water from other sources. Independent of the exact schematic of the water sampling system, the OWM and IWM modules of SWIM analyze the same water sample from a single input source. For both OWM and IWM, electronics to power and control the subsystems is required along with the separation and detection hardware. SWIM system level power and data handling will be included in the system design.

A more detailed sample and analysis flow is illustrated schematically in Figure 2. Water samples are supplied to the system and could be sourced from a connection to the potable water bus similar to what is done for MiniTOCA[6] or could be provided using sample bags, which is standard practice for operating TOCA and MiniTOCA. An interesting source of water for analysis on ISS would be humidity condensate. The condensing heat exchanger is part of the water recovery system, and in the process of condensing humidity in the cabin also condenses organics that may be present in the air. The schematic shows the water sample traveling to OWM and IWM sampling points before being routed to a waste container. OWM and IWM will sample the same water sample, but report results according to their different analytical capabilities.

As illustrated in Figure 2, OWM is a GCMS system. The injection, separation, and detection sections of OWM are shown in block diagram form. Project-developed pneumatic controls supply GC carrier gas to the injector, which injects the water sample onto the separation column. The GC will need a source of carrier gas. After column separation, detection by flame ionization detection (FID), thermal conductivity detection (TCD) and mass spectrometry can occur. The detection section of OWM requires low voltage, high voltage, and radio frequency electronics. OWM electronics will interface back to the SWIM main control electronics as is shown conceptually in Figure 1.

The IWM section comprises a block of physical properties monitors and ion selective electrodes, followed by the CE-C4D section. The pH, conductivity, and ISEs can be thought of as "online" detectors. The separation science portion of IWM occurs in the CE separation section. A high voltage supply biases the end of two separation capillaries using opposite polarity biases, shown as the circled "plus" and "minus" on the diagram. Positively charged and negatively charged ionic species are detected at the end of the respective CE capillaries with separate C4D detectors. The capillary shown between the two detectors is to complete the electrical biasing circuit using the working fluid as the conducting medium. IWM requires some reagents (CE mobile phase electrolyte) and will generate some waste.

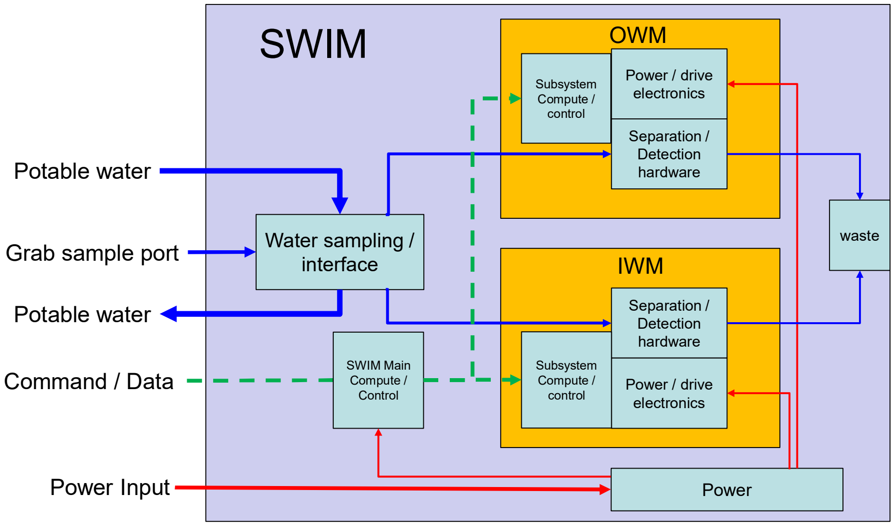

Figure 1. Block diagram of the SWIM system. Water could be sampled from multiple locations such as the potable water bus, or other locations using grab sample bags. The water sample is routed to OWM and IWM for chemical analysis. The OWM and IWM hardware will require command / data / control electronics for the analytical hardware that is used. Some waste water is expected to be produced.

III. Chemical Target Lists

SWIM subsystems OWM[7] and IWM[8] have previously presented lists of chemicals/species of interest for detection. These compounds, ions, or metals all have relevance to potable water quality or water quality for the safe and correct operation of spacecraft systems. Work continues on definition of the required chemical targets for SWIM, and a current listing of required species to measure with SWIM is shown in Table 1 below.

The required compounds to measure are sourced from requirements documents for ISS as well as from stakeholder inputs. Requirements documents include SSP 41000, System Specification for the International Space Station, SSP 50260 International Space Station Medical Operations Requirements Document (MORD), and JSC 63414 Spacecraft Water Exposure Guidelines (SWEG).

The majority of the chemicals in the organic column come from the SWEG. Ethanol, isopropanol, methyl sulfone, trimethylsilanol, benzyl alcohol and o-phthalaldehyde were added as a result of stakeholder inputs to the project. Those organics are of special interest for ISS because they are historically observed on ISS in humidity condensate or present an interesting system diagnostic / consequence. Ethanol and isopropanol, for example, are commonly used for cleaning of spacecraft parts and may be present at higher concentration in atmospheres of visiting vehicles or due to other ISS operations. Some of the chemicals on the list also appear in water quality requirements for Russian segment water. Formaldehyde is listed as an organic detection goal because GCMS without sample preparation is atypical for determination of formaldehyde in water.

The choice of GCMS for organics detection matches the state of the art and standard practices for water analysis. Environmental Protection Agency (EPA) methods 524, 624, 8260, and 8270 are GC- and GCMS based methods for complex organic mixtures and many OWM chemical targets are listed in these methods. The TEC lab utilizes GCMS as part of their analysis sequence on returned water samples. We expect that given the wide range of chemical functionalities included in the OWM target list that designing SWIM to detect the listed range will lend itself to future characterization of unknowns, if they occur. GCMS for organics has space flight heritage, a recent relevant example being Spacecraft Atmosphere Monitor (SAM),[9] which is currently an ongoing technology demonstration project.

Carbonate and bicarbonate are of interest to the SWIM project and are listed as inorganic detection goals. Motivation for detection includes that they comprise the total inorganic carbon (TIC) component of the water, as well as bicarbonate being a filtration bed breakthrough product. Knowledge of TIC can be important for understanding TOC measurements. TOC analyzers such as TOCA and MiniTOCA are designed to measure total organic carbon in the presence of TIC, but do not report the TIC value directly. Determining the value of TIC present when a TOC measurement is made allows better understanding of the detected TOC value and total carbon accounting for the water sample.

Table 1. List of chemicals of interest for SWIM. Those marked in asterisks are detection goals.

Organics	Inorganics
acetone	potassium
methyl ethyl ketone	calcium
methanol	magnesium
isopropyl alcohol	chloride
ethanol	nitrate
dichloromethane	sulfate
trimethylsilanol	ammonium
benzene	barium
chloroform	manganese
propylene glycol	nickel
ethylene glycol	silver
benzyl alcohol	zinc
phenol	chromium
dimethylsilanediol (DMSD)	cadmium
caprolactam	lead
methyl sulfone	iron
o-phthalaldehyde	copper
di-n-butyl-phthalate	antimony
2-mercaptobenzathiazole	formate
n-phenyl-beta-naphthylamine	iodide
di(2-ethylhexyl) phthalate	carbonate*
formaldehyde*	bicarbonate*

A key feature of SWIM is determination of unknowns or new chemicals which appear in the water that is analyzed. The technology is capable of this because the separation science approaches used are generalized for chemcals that would be present. We expect that if other organics or inorganics are present in water samples, SWIM will be capable

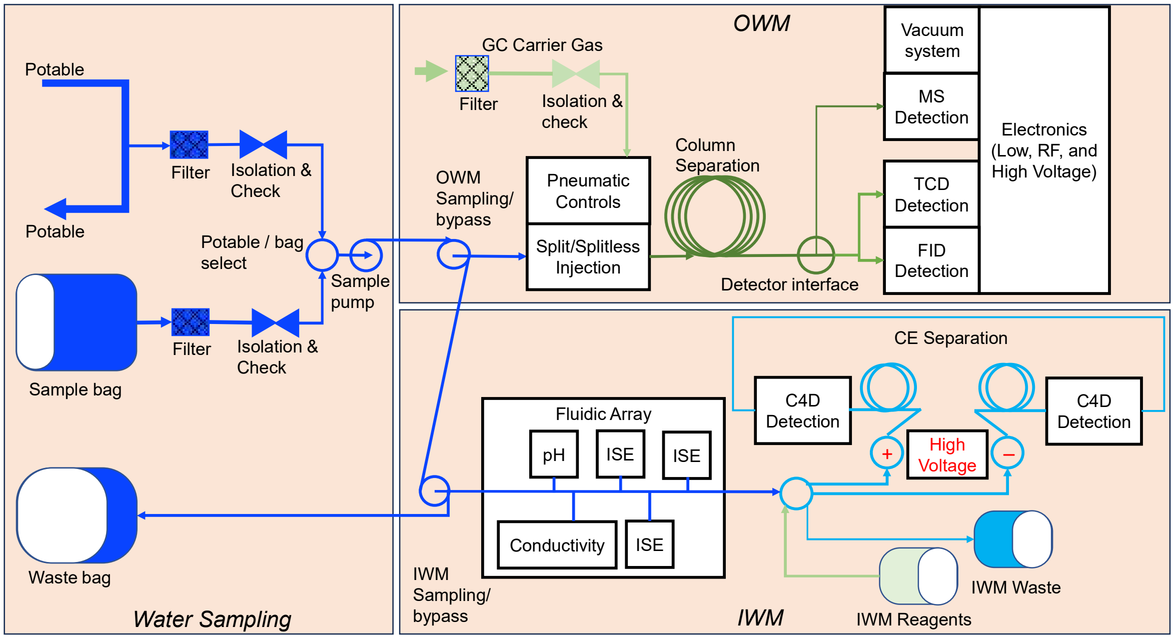

Figure 2. SWIM system schematic showing water sampling, OWM, and IWM sections of the system.

of identifying those. Examples include any variety of alcohols or ketones present in a water sample. After GC separation of the mixture, mass spectrometry will be able to uniquely identify which alcohol or ketone it is. The same situation occurs with inorganic analysis. Ions such as sodium, bromide, or phosphate are in-family with the species normally measured by IWM using CE-C4D and are not actively excluded from detection by SWIM. If those species are present, they would be detected. For the GCMS and CE-C4D functionalities of SWIM, there is not a specific detector or collector per chemical. The detectors are non-specific, which is why they were chosen. It is possible to use a non-specific detector when the mixture is pre-separated.

IV. Forward work and Project Plans

We presented previously on technology development efforts for OWM and IWM, and the subsystems continue technology maturation efforts. Planned development efforts in support of exploration goals include a custom compute element for SWIM which leverages previous development of radiation hardened computing architecture that was developed at NASA Jet Propulsion Laboratory (JPL) for planetary missions. The radiation environment for exploration missions will be more demanding than LEO applications. Ionizing radiation factors into electronics design, and so having a command and data handling (C&DH) compute element which is already ruggedized is an advantage. This is difficult to achieve using COTS, because the computing power requirements for SWIM are fairly demanding. Radiation hardened computers currently available are old designs and would “box-in” the capabilities of SWIM. A more modular architecture for the compute element is suited to future implementations.

To support radiation tolerance and design flexibility for other subsystems apart from the C&DH element, SWIM plans to have a philosophy of minimizing COTS devices having processors or embedded computing in favor of lower level implementation of these functions. This philosophy will be applied to the technology demonstration project where possible, which will set the hardware design in the right direction for future implementations. The motivations for this low-level implementation approach include future flexibility in electronics parts selection and ability to tailor future designs to be radiation tolerant. An example of this on OWM is the pressure and flow control hardware for controlling the carrier gas in the gas chromatograph section of SWIM. COTS mass flow controller and pressure controllers are widely available and widely used for GC and other applications. Each of these has a microcontroller running vendor firmware which provides the physical control over the sensors and valve packaged in the flow controller or meter. Even in LEO applications, COTS hardware presents challenges in the areas of obsolescence and supply chain. SWIM has built and tested simple, robust pressure control for the GC from component parts. Control loop and processing comes from a microcontroller we selected which has a known radiation hardened version. Pressure sensors are driven and read out by project-developed electronics circuits. For IWM, development of miniaturized multiport valves and actuators for those valves has taken place. Already as part of the initial concept development for some of the IWM components, the designs were implemented “flight forward” in terms of radiation tolerance because they were originally developed for planetary missions to Mars or outer planets where the radiation environment is more severe than in LEO.

The SWIM project is preparing for a System Requirements Review (SRR) in Summer 2025. Following requirements baselining, as a part of preliminary design activities, architecture studies will be completed to further define the instrument schematic. For IWM, we will need to determine how best to implement the measurement sequence for inorganic species. Referencing Figure 2, the exact plumbing routing for pH, conductivity sensors, and ISEs is forward work because if SWIM has a direct connection to the potable water bus, it may be desirable for higher frequency or “constant” monitoring of physical properties such as conductivity. There are complexity consequences due to this type of architecture. It could be that SWIM must be built so that sections can operate powered constantly and other sections powered on on-demand. Other decisions to make are regarding OWM detectors. While GCMS will be required, the exact use cases and interface for the FID and TCD detectors will need to be further defined. It is possible one of those detectors will be included in SWIM differently than is shown in Figure 2. On the subject of required chemicals to detect, more feasibility studies will be performed for the detection goal chemicals. Capability for detection of dissolved formaldehyde without sample prep or derivatization will be determined. A study on detection of carbonate and bicarbonate with IWM technologies is planned.

Acknowledgments

The work described in this report took place at NASA Johnson Space Center in the Crew and Thermal Systems Division, Life Support Systems branch with support from KBR as part of the Human Health and Performance Contract, HHPC (NNJ15HK11B); and at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration (80NM0018D0004).

The project gratefully acknowledges advocacy and funding support from the NASA Mars Campaign Office (MCO) Life Support Systems (LSS) project.

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