

# Dialysis-based Passive Biocide Delivery System: An Exploratory Analysis on the Development of a Silver Dosing Alternative for Spacecraft Potable Water Systems

Rogelio E. Garcia Fernandez<sup>1</sup> and Robert R. Beitle, Jr.<sup>2</sup>  
*University of Arkansas, Fayetteville, Arkansas, 72701*

**This paper describes the use of a dialysis-based passive dosing system for silver ion delivery as a biocide for potable water systems in spacecraft and extraterrestrial bases. A silver dosing device has been developed for continuous water treatment, based on the International Space Station Water Processor Assembly framework. The Passive Biocide Delivery System is designed to supply a stream of product water with silver ions at a concentration range of 200-400 ppb, using a membrane to control dosing. Potable water with these silver concentrations can be safely consumed by humans. The dialysis approach is attractive since it does not require additional energy nor high pressure to function. Computational Transport Phenomena has been implemented to study the performance of the membrane setup at particular operational conditions and guide the choice of membrane properties. The results suggest that the dosing device can release silver ions at the target levels for at least eight hours without excessive silver salt consumption. This paper contains technical background and preliminary results from the Passive Biocide Delivery System development and presents the benefits and challenges of its implementations in spacecraft and Lunar/Martian bases.**

## Nomenclature

$C_{Ag+,c}$	=	Initial Silver Ion Concentration in Sample Chamber
C.E.	=	Cellulose Ester
$D_{Ag+,w}$	=	Silver Ion Diffusion Coefficient in Water
DI	=	Deionized
E.C.	=	Electroconductivity
ESIG	=	Electrolytic Silver-Ion Generator
H	=	Partition Coefficient
ISS	=	International Space Station
IXB	=	Ion-eXchange Bed
LFFM	=	Laminar Fluid Flow Module
LSS	=	Life Support System
MCV	=	Microbial Check Valve
MWCO	=	Molecular-Weight Cutoff
NASA	=	National Aeronautics and Space Administration
$P_{Ag+,m}$	=	Silver Ion Permeability in Membrane
PBDS	=	Passive Biocide Delivery System
ppb	=	Parts Per Billion
TDSM	=	Transport of Diluted Species Module
TOC	=	Total Organic Carbon
WPA	=	Water Processor Assembly
WRS	=	Water Recovery System

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<sup>1</sup> Graduate Student, Ralph E. Martin Department of Chemical Engineering, 3202 Bell Engineering Center, Fayetteville, AR 72701-1201

<sup>2</sup> Associate Vice Chancellor for Research and Innovation, Ralph E. Martin Department of Chemical Engineering, 3202 Bell Engineering Center, Fayetteville, AR 72701-1201

## I. Introduction

Space has become the last exploration frontier for humanity, uniquely challenging scientists and engineers to design innovative technologies to explore it better. The environmental hostility that space destinations (planets and moons) offer to humans challenges critical field research. Even though cutting-edge technologies, such as partially or fully autonomous rovers, have been developed to perform field research and exploration on other celestial bodies, these tasks could be performed more adequately and meticulously by on-the-ground scientists. Bringing more scientists into space, the Moon, and Mars, requires not only efficient engineering and safe transportation but also environmental life-support systems that can maintain provisions, air, and water, especially for extended missions.

A Life Support System (LSS) is an ensemble of devices and structures that ensure the conditions inside a spacecraft or base necessary for living, such as drinking water, oxygen, hygiene, food, waste disposal, ionizing radiation protection, and thermal insulation.<sup>1</sup> The Water Recovery System (WRS) collects, filters, purifies, and sterilizes water. In general, the goal of a WRS is not only to store water but also to produce drinking water from non-potable sources, particularly washing water, flushing water, fecal fluids, urine, and exhaled breath condensate. A WRS involves heating/cooling, chemical treatment, deionization, gas-liquid separation, filtration, and disinfection to recycle water from available resources. Recycling water in a spacecraft or an extraterrestrial base is crucial since launching water to space results in a costly operation. In the last decade, the cost of sending one kilogram of cargo to low earth orbit has ranged from \$34,500 to \$1,500 (U.S. dollar cost estimates in the fiscal year 2021).<sup>2</sup> Furthermore, it is estimated that crewmembers consume a minimum of two liters of water per mission day only for drinking.<sup>3</sup> Therefore, current and future crewed missions need to rely on water recycling processes to minimize operational expenses.

A WRS would generally operate in a semi-continuous manner mainly for two reasons. First, there would not be a volumetrically sufficient continuous source of used water in a spacecraft to have a fully continuous WRS. Second, a semi-continuous process can be automated to a high degree, allowing astronauts to focus on other tasks. A batch WRS would require several steps to be performed separately by the crew. Thus, if a semi-continuous WRS design is an attractive configuration, enough raw water must be collected in the spacecraft or base before the startup. The analysis that is presented here is based on a semi-continuous operation.

Typically, the last step in the water treatment and recycling process is to add a biocide to the product water to prevent microbial growth. Although all bacteria would be killed in a WRS's intermediate stages (e.g., heaters and reactors), there would be an inevitable amount of total organic carbon (TOC) in the product water that can allow microorganisms to grow. Consequently, biocide addition is an appropriate action. Since the biocide only has a preventive objective and its dosage should not require additional power, the biocide system is referred to as "passive." The Apollo missions contemplated using ionic silver ( $\text{Ag}^+$ ) as a biocide, while Skylab, the Shuttle program, and the International Space Station (ISS) adopted iodine.<sup>4-7</sup> The National Aeronautics and Space Administration (NASA) has reconsidered the implementation of silver biocide instead of iodine for long-duration space missions due to iodine's performance on the ISS. The iodine treatment has been successful on the ISS; however, the crew has to remove the biocide from the product water before consumption. Iodine can cause thyroidal problems if iodine-containing water is consumed.<sup>8</sup> In contrast, a silver biocide can effectively inhibit microbial growth at concentrations that are safe for humans to consume. The human body excretes 90% of silver ions when ingested at low concentrations (i.e., 500 ppb).<sup>9-11</sup> If future space missions adopt a semi-continuous WRS and silver as a biocide, a passive biocide dosing system (PBDS) will be an indispensable WRS component. Thus, addressing the technical necessities in designing an efficient WRS for spacecraft or extraterrestrial bases, a unique design for a PBDS has been formulated by exploring the capabilities of dialysis as biocide dosing mechanisms.

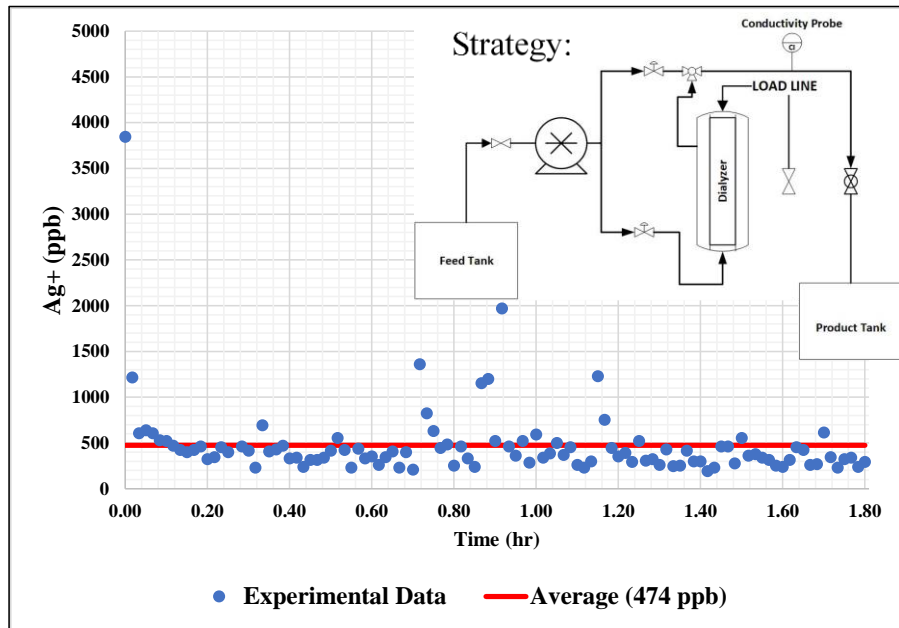
## II. Background

This work originates from a task developed by NASA for the 2019 Waste-Management Education and Research Consortium at New Mexico State University (Las Cruces, New Mexico). NASA challenged undergraduate university teams to develop a silver-ion dosing technology that conformed to the following criteria:

- Add silver ions at a concentration range of 300 to 500 ppb to a stream of deionized water flowing at 0.1 to 0.15 L/min.
- Operate at ambient temperature and pressures up to 30 PSIG.
- Operate at pH ranges between 4.5-9.0.
- Weigh less than or equal to 5kg.
- Be small, robust, easily maintainable, and be capable of working in microgravity.

Beitle. et al. continuously processed five gallons of deionized (DI) water at the required flow rate and demonstrated that a dialysis cartridge coupled to a bypass could dose silver ions at the target level, with the competition results

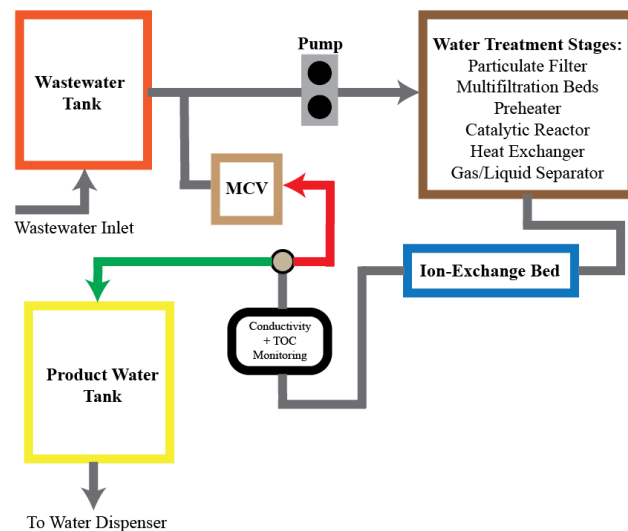
expanded herein.<sup>12</sup> Their results and strategy are shown in Figure 1.<sup>12</sup> In early 2020, NASA released a Small Business Technology Transfer solicitation of technologies for delivery, maintenance, and monitoring silver in potable water. This solicitation provided a new silver-ion concentration criterium for the dosing technology: from 200 to 400 ppb. Additionally, NASA asked<sup>13</sup>, “the technology should also be capable of providing continuous, stable and autonomous operation, and be fully functional following periods of long-term system dormancy – up to 1 year.”



**Figure 1: Silver Ion Release Data from Beitle. et al.**<sup>12</sup> The system utilized a dialyzer to dose silver ions to a stream of DI water and required a manually-controlled bypass stream to regulate the output when this was off-target. The bypass diluted the output level to the required concentration.

Silver ions are cell lysis initiators; ergo, their biocide nature. When the positively charged silver ions interact with the negatively charged lipids of microorganisms, cell lysis is initiated.<sup>14</sup> The pathogens die by cell rupture. Presumably, the first silver-based dosing technology was the electrolytic silver-ion generator (ESIG) developed for the Apollo missions. The in-line ESIG consisted of a cell with a silver anode that discharged silver ions to the water when a voltage was applied; the technology was never deployed during flight.<sup>4</sup> Ultimately, iodine-based technologies became the choice for subsequent space missions.

The best example of the PBDS deployment is in the ISS. Two iodine-based pieces of equipment were implemented on the ISS WRS, the Water Processor Assembly (WPA): an ion-exchange bed (IXB) and a



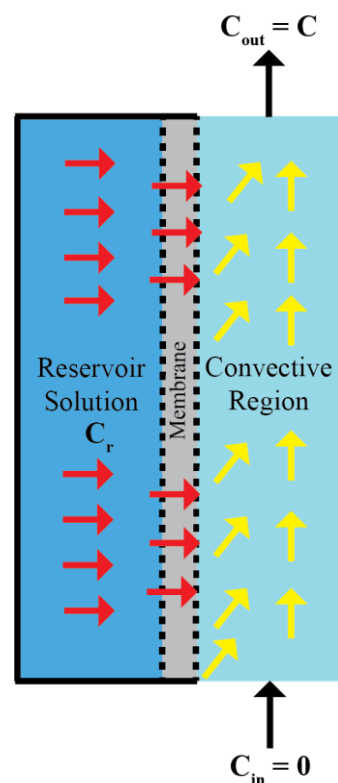
**Figure 2. The International Space Station (ISS) Water Processor Assembly (WPA), simplified schematic.**<sup>15</sup> The Passive Biocide Delivery System (PBDS) is an iodine-based ion-exchange bed. When the product water does not meet the requirements, it is redirected back to the first stage of the water treatment process.

Microbial Check Valve (MCV) (see Figure 2).<sup>15,16</sup> The WPA has a recirculation setup; the water that does not pass the quality monitoring is redirected to the system's first stage. The IXB supplies iodine ions to the treated water after absorbing undesired cations and anions from previous water-treatment steps. The IXB is the PBDS in the WPA. On the other hand, the MCV prevents backflow contamination by microorganisms from the raw water on the recirculation line with minimal iodine stripping. As Figure 2 shows, although the wastewater does not reach the product water due to the flow direction, microorganisms can propagate from the wastewater to the product water. Therefore, the MCV is placed on the recirculation line to avoid any biological contamination. If a silver-based PBDS is to be implemented in a WRS similar to the ISS WPA, the system would replace the IXB and require a silver-based MCV.

Even though the iodine-based system has been successful, the iodine in the product water must be removed from the water before being consumed due to its health effects. Moreover, the U.S. ISS water system is not compatible with the Russian system, which uses silver. The Russian team manually adds a silver species to their potable water before sending it to the ISS.<sup>17</sup> If water from the ISS Russian section mixes with water from the U.S. side, silver iodine precipitation may occur. This precipitate does not have any biocidal properties and could cause flow stoppage in the system.<sup>18</sup> Therefore, silver has to be added to the water after iodine is filtered to keep bacterial inhibition and make the water compatible with the Russian supply (sharing water in space may be crucial in some circumstances). Furthermore, the removal of iodine on the ISS employs an activated carbon-ion exchange bed connected to the water dispenser, reducing the iodine level to low concentrations that meet the 1 mg/day iodine intake limit for humans.<sup>18</sup> Consequently, the iodine-based PBDS increases the ISS WPA complexity.

If future lunar or Martian crewed missions adopt a system like the ISS WPA, a silver-based PBDS could benefit the spacecraft WRS design. Nevertheless, not many in-line silver-based PBDS technologies have been specifically developed for this application. The more promising technology is ESIG, whose most recently-reported downsides include: its size-dependency, requirement of very-low conductivity water, and pH-dependent electrode fouling.<sup>19</sup> Although periodic cleaning of the electrode surface and polarity reversal can reduce the generation of resistive oxide layers,<sup>20</sup> this procedure raises maintenance. One promising passive silver biocide dosing system currently under development consists of a polyurethane composite foam loaded with silver chloride nanoparticles and packed into a cartridge.<sup>8,21</sup> When water flows through the cartridge, silver ions are released via dissolution. As of March 2021, results from flow-through tests have only been published for short-term experiments (10 minutes), showing a silver release below the 200 ppb required minimum.<sup>22</sup>

Our work further explores the PBDS via dialysis. Dialysis is a process of selective diffusion through a membrane by dissolved solutes. Unlike other membrane processes, only solutes move across the membrane in dialysis with minimal / no solvent exchange. Dialysis is typically used to purify fluids by inducing contaminant migration to another fluid in which its concentration is lower according to Fick's Law. This dialysis principle can also be used to accomplish an opposite goal: dosing or imparting a solute into a purified water stream. Therefore, a PBDS could be developed using dialysis as the biocide delivery mechanism. In other words, a dialyzer can be repurposed to serve as a PBDS. Two formats could be chosen: steady-state dialysis or unsteady-state dialysis. Unsteady-state dialysis was selected for this study since the proposed design requires less instrumentation and orchestration operating transiently than at steady-state. Unlike a steady-state dialyzer (counter flow streams separated by a membrane), an unsteady-state dialyzer only has one convective region. Figure 3 illustrates the solute release in dynamic dialysis.

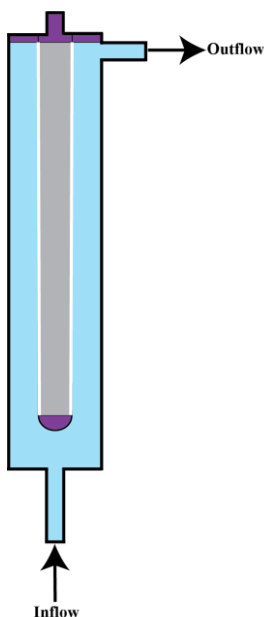


**Figure 3. Solute Release in Dynamic Dialysis.** *The solute travels from the reservoir solution to the convective region due to the existing concentration difference between them. The solute release slows when the reservoir's concentration is not sufficient to establish a driving concentration gradient. The red arrows indicate diffusive transport, and the yellow arrows show diffusive and convective transport. The black arrows show the solvent flow direction, in this case treated water.*

Unsteady-state dialysis is a mass-transfer process that is intrinsically transient. The release slows when the reservoir solute concentration is too low to drive a concentration gradient. An active layer supplies solute to the diffusion process at the interface between the reservoir solution and the membrane. In this active layer, a depletion zone is created by the diffusive gradient. When this depletion zone reaches the active layer's size, the release rate drops.<sup>23</sup> As Figure 3 shows, the solute diffuses from the reservoir solution to the membrane and then reaches a convective region. As soon as the solute crosses the membrane, the receiving solution's perpendicular flow removes the solute from the system.

The solute can diffuse through the membrane since the membrane is filled with solvent. However, minimal solvent is exchanged between the reservoir solution and the convective region when the reservoir solution's static pressure equalizes with the flowing fluid's pressure. Both sides fill the membrane's free volume with solvent creating a bridge for the solute. Additionally, the membrane's porosity must be large enough to allow the solvent molecules to enter. The solute diffuses through a liquid phase in an interconnected tortuous path in the solvent-swollen membrane.

To test this concept, silver ions can be dosed to a stream of DI water using the reservoir delivery setup shown in Figure 1. This study employs a dialyzer that encloses an interior chamber in which a concentrated silver salt solution is loaded. This sample chamber is a cylindrical dialysis bag made of semi-permeable biotech-grade Cellulose Ester (C.E.) membrane tubing. Between the dialyzer's housing and the sample chamber, there is an annular space through which the process fluid flows. Figure 4 displays the dialyzer's layout. As soon as the DI water enters the annular space and is in contact with the membrane, the mass transfer from the sample chamber to the flowing DI water begins. Since the silver-salt solution would be highly concentrated and the membrane's molecular-weight cutoff (MWCO) would be optimally small, a slow silver release rate would be expected, and the maintenance required to replenish the system would be low. The slow-release rate would allow the supply of silver ions to the overall water recovery processing time while maintaining the PBDS's operability for months. For instance, the overall water recovery process would take eleven hours at a hundred milliliters per miniature volumetric flow rate based on the ISS WPA's 68-liters wastewater tank volume.<sup>15</sup>



**Figure 4. Dialyzer's Two-dimensional Layout.** *The process fluid (deionized water) enters the device through the bottom inlet and exits at the top outlet. This self-contained device incorporates a semi-permeable membrane tubing (white interior borders) that separates the sample chamber (grey area) from the surrounding annular flow-through chamber (light blue area). The port (purple top cap) provides easy access for loading the silver solution to the inner chamber. The interior end cap (purple) provides support to the membrane against the inlet's flow. Silver ions are delivered to the deionized water as it flows around the membrane.*

The dialysis-based PBDS's performance was investigated for the following reasons: 1) the dialyzer is a lightweight device (< 100 grams); 2) water can flow through the dialyzer with negligible pressure drop; 3) the biotech-grade cellulose acetate membrane can tolerate 2-9 pH levels; 4) dialysis transport phenomena do not depend on gravity; 5)

the dialyzer has a modest size (2.2 cm x 45 cm); 6) the dialyzer does not require additional power to operate making it a passive dosing system. Computer modeling and experimental testing evaluated the efficacy of silver ion release by the dialyzer. The results indicated if the dialysis-based PBDS is a feasible method for delivering and replenishing silver ions in spacecraft or extraterrestrial bases potable water systems and informed us to choose membranes better on the needed permeability to satisfy the ppb requirement.

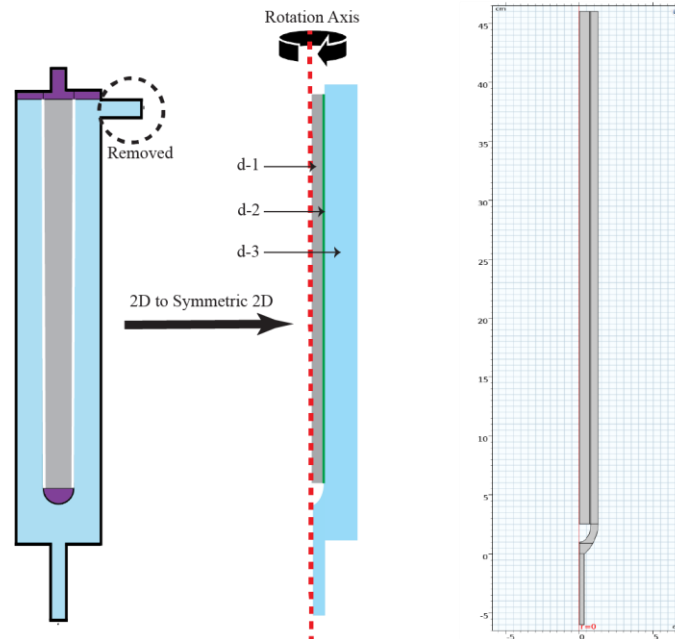
### III. Materials and Methods

The methodology adopted to study the dialysis-based PBDS technology involves computer modeling to evaluate and parametrize the dialysis system and experimental testing to assess an available dialyzer. This investigation intends to determine whether the dialysis-based PBDS can supply silver ions to a stream of DI water, at 200-400 ppb levels for the time it takes to process 70% of the ISS wastewater tank's volume at 100 mL/hr volumetric flow rate.

#### A. Computer Modeling

The dialysis system was modeled using COMSOL Multiphysics® version 5.5 software.<sup>24</sup> This software provides conventional physics-based user interfaces and coupled systems of partial differential equations. The modeling workflow encompasses five steps: geometry design, material selection, physics implementation, and study type. Moreover, modeling dialysis requires incorporating more than one physical principle: fluid flow and solute transport.

Since the dialyzer has a vertical symmetry axis (omitting the lateral outlet shown in Figure 4), the computational model can be simplified by representing the dialyzer with a two-dimensional symmetric geometry. This technique makes the simulation computationally less expensive, allows a more convenient allocation of spatial boundary conditions, and provides three-dimensional visualizations. Figure 5 shows the geometrical representation of the dialyzer for the COMSOL Multiphysics® model. The lateral outlet connector of the original dialyzer was removed from the COMSOL Multiphysics® geometry to make the resolution of the two-dimensional-symmetric plane possible. Therefore, the outlet of the system will be at domain-3's top edge in the computer model. The study only includes domains where transport phenomena are significant. Hence, the dialyzer's interior and exterior housing components are not included in the geometry; however, their effects are added by boundary conditions.



**Figure 5. Two-dimensional Symmetric Geometry for Computational Model.** The symmetric geometry only includes domains where transport phenomena occur. Domain 1 (d-1) refers to the sample chamber (grey area). Domain 2 (d-2) refers to the membrane (green line). Domain 3 (d-3) refers to the convective region (light blue area). The housing components are not drawn in this geometry since they can be modeled as boundary conditions. The rotation axis allows generating a three-dimensional visualization from the results.

Liquid water was selected as the material for all domains. Although the membrane's material is intrinsically essential in the analysis, liquid water was also chosen for the domain corresponding to the membrane. In this analysis, the membrane's domains corresponded to the liquid phase in an interconnected tortuous path in the solvent-swollen membrane. However, the tortuous path (or network) was not explicitly drawn in the geometry; instead, the tortuous path's diffusive restriction was included by specifying a constant and isotropic solute permeability coefficient in the membrane's domain. Furthermore, the properties of liquid water were set for room temperature (25°C).

Two physics principles modules were applied to the transport phenomena simulation: The Laminar Fluid Flow Module (LFFM) and the Transport of Diluted Species Module (TDSM). The LFFM was used in the study since the flow regime is laminar according to the device's geometry and the volumetric flow rate (inlet's Reynolds number ~ 334). The TDSM was selected since the silver ion concentration is expected to behave as a dilute solute in a solvent and water is clearly identified as the solvent, and the main transport mechanisms are diffusion and convection. The modules were executed separately since the fluid flow was stationary, whereas the solute transport was time-dependent. Additionally, the LFFM was carried out first since the TDSM requires inputs from the fluid flow study. The LFFM was only specified in domain-2 because it is the only forced-convective region, while the TDSM was defined in all the domains since solute transport occurs everywhere. Equations (1) and (2) are the partial differential equations from the LFFM and the TDSM, respectively. Eq. (1) is derived from the Navier–Stokes equations, while Eq. (2) is based on mass conservation.

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F} + \rho\mathbf{g} \quad (1)$$

$$\nabla \cdot (-D\nabla C_{Ag+} + C_{Ag+}\mathbf{u}) = \frac{dC_{Ag+}}{dt} \quad (2)$$

The main parameters for the LFFM were the water's physical properties and the dialyzer's inlet velocity and outlet pressure. The gravitational acceleration term was set to both zero and 9.81 m/s<sup>2</sup> (two analyses). The TDSM was only used to model the transport of the silver ions. The counterion was not included in this model's chemical species since the simulation only sought to predict a simple release behavior. The fundamental parameters for the TDSM were concentrations and diffusion coefficients. A 1.648x10<sup>-9</sup> m<sup>2</sup>/s value, which corresponds to the silver ion's aqueous diffusion coefficient at infinite dilution, was used as the silver ion's diffusion coefficient in the sample chamber and the convective region.<sup>25</sup> In domain 2 (the domain corresponding to the membrane), a different solute diffusion (permeability) coefficient was designated. It was assumed that the solute's permeability in the membrane should not depend on the Reservoir solution's concentration in isothermal operation at constant membrane thickness and fluid viscosity. Hence, the solute's permeability in the membrane must also have a fixed value. According to Eq. (3), the solute's permeability ( $P_{Ag+,m}$ ) is equal to a dimensionless partition (solubility) coefficient (H) multiplied by the solute's diffusion coefficient in the solvent ( $D_{Ag+,w}$ ).<sup>26,27</sup> Instead of determining "H" experimentally, this constant was parametrized in the simulation to a value that provided the desired silver ion release. It was assumed that the permeability's magnitude had to depart from  $D_{Ag+,w}$ . Therefore, the partition coefficient (H) was preconditioned to take values from 0.1 to 0.0001. Additionally, the sample chamber's initial silver ion concentration ( $C_{Ag+,c}$ ) was also parametrized to have 50 mol/m<sup>3</sup>, 100 mol/m<sup>3</sup>, 500 mol/m<sup>3</sup>, and 1000 mol/m<sup>3</sup> values.

$$P_{Ag+,m} = H D_{Ag+,w} \quad (3)$$

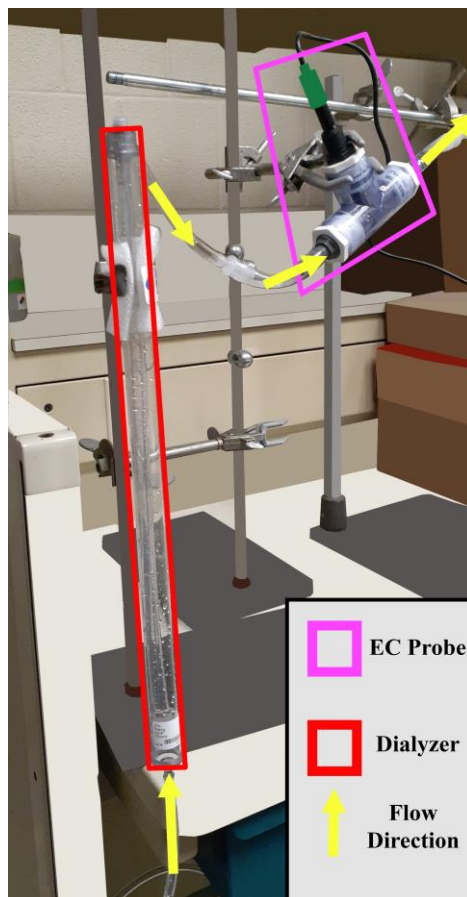
Physics principles controlled meshes were generated for both modules. The mesh sizes are based on the local dimensions from the model's geometry. The LFFM required a normal size mesh, whereas an extra-fine mesh was utilized for the TDSM. These mesh sizes provided the least numerical error.

## B. Experimental Testing

The dialysis system was tested by loading the dialyzer's sample chamber with a concentrated silver solution and running DI water through the dialyzer. Electroconductivity (E.C.) measurements were taken at the dialyzer's outlet to determine the silver ion output. The silver solution concentration loaded in the dialyzer's sample chamber was determined from the COMSOL Multiphysics® simulations. According to the literature, the most appropriate silver

salts for this application are silver chloride, silver carbonate, and silver nitrate.<sup>8,21,28,29</sup> Silver lactate was utilized in this experiment because of its chemical safety and availability. The goal of the experiment is to measure the silver release by the dialysis system and compare it with the simulations. Figure 6 shows the experimental setup.

The dialyzer has an MWCO range of 0.1 - 0.5 kilo-Daltons, which provides a relative pore size big enough for inorganic salts to pass. The DI water was generated using an EVOQUA Deionization Systems (Pittsburgh, Pennsylvania). Forty-eight liters of DI water were accumulated for each experimental run. The E.C. measurements were taken using an Atlas Scientific© conductivity probe with a 0.1 cell constant (Long Island City, NY). The E.C. probe's calibration was developed with the Hanna Instruments© HI96737 Silver Portable Photometer (Smithfield, Rhode Island).



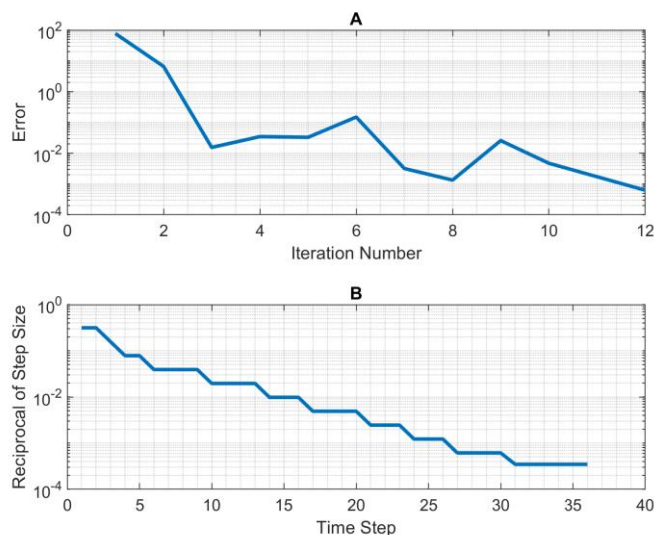
**Figure 6. Dialysis-based Passive Biocide Delivery System Experimental Setup.** *The dialyzer is initially loaded with a concentrated silver solution. Then, deionized water is pumped through the dialyzer at a volumetric flow rate of 100 mL/min. As the flowing water is in contact with the dialysis membrane, silver ions are released. Electroconductivity measurements are taken at the dialyzer's outlet to estimate the silver ion concentrations. The red box and the magenta boxes indicate the dialyzer's location and the electroconductivity probe, respectively. The yellow arrows show the flow's direction.*

The dialyzer was tested three times with the same silver solution concentration and volumetric flow rate. The experimental apparatus was covered to prevent light exposure since silver lactate is sensitive to light and can precipitate from the solution.<sup>30</sup> No more than one dialyzer was tested at the same time (in a parallel configuration). Each run took approximately eight hours to complete. After each test, the concentrated silver solution was withdrawn from the dialyzer's sample chamber, and the dialyzer was stored with both the sample and annular chambers filled with DI water. Before the dialyzer was recharged, the sample chamber was flushed with DI water to remove any visible precipitate particles.



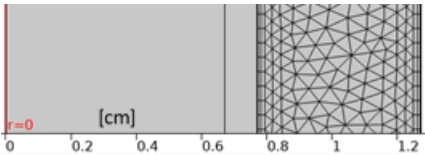
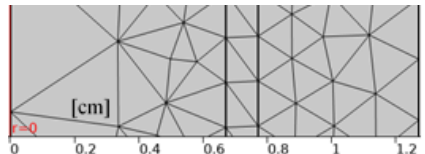
#### IV. Results & Discussion

The numerical error and convergence for the COMSOL Multiphysics® model are summarized in Figure 7 and Table 1. Plot-A shows the numerical error from the LFFM, while plot-B shows the convergence from the TDSM. These modules have different numerical solver assessments since the LFFM was a stationary analysis, whereas the TDSM was a transient one. The LFFM and the TDSM took 12 iterations and 36 time-steps, respectively. Furthermore, the mesh, mesh size, and the physic principles validation (mass/mol balance) are compiled in Table 1. A small segment of the meshed geometry (as illustrated in Figure 5) is shown in Table 1 for illustrative purposes, and the local mesh sizes should not be compared between modules since they are generated independently within their module. The geometry has partial mesh for the LFFM since fluid flow physic only occurs in that meshed region. The 4.19% absolute error obtained from the TDSM could not be avoided by using other physics-controlled and attended user-based meshes. This error was concluded to be irrelevant since the goal was to visualize and understand the release process exploratorily.



**Figure 7. Error and Convergence from the COMSOL Multiphysics® model.** Plot-A shows the numerical error from the LFFM, while plot-B reports the convergence from the TDSM.

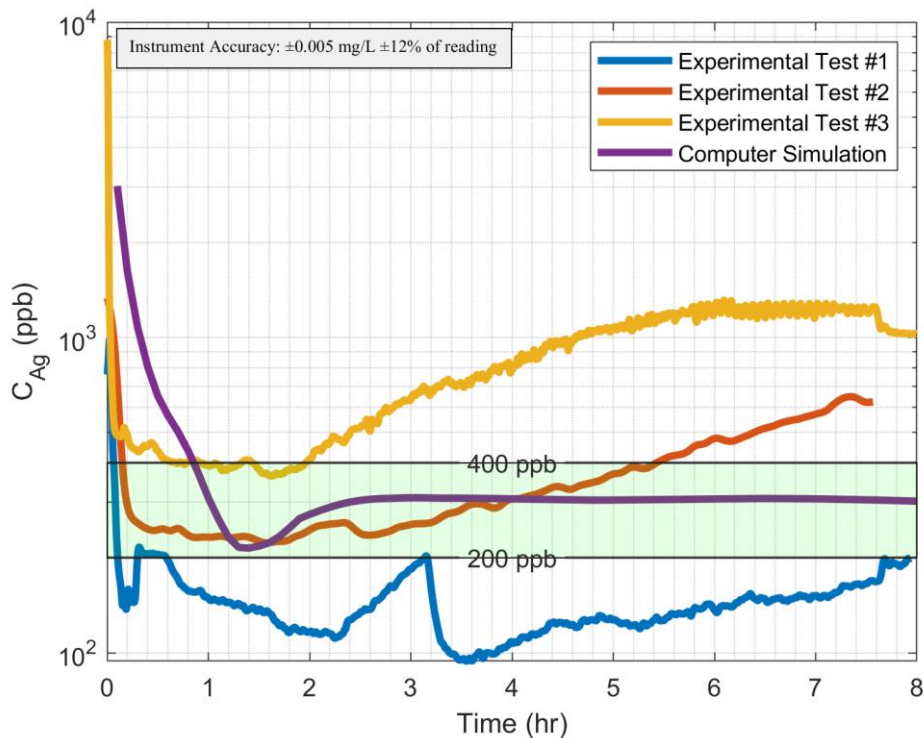
**Table 1. Computer Simulation Performance**

Physics Module	Local Mesh Size	Mesh	Mass/Mol Balance		Error
			IN	OUT	
LFFM	Normal		0.0016637 kg/s	0.0016637 kg/s	0.00%
TDSM	Extra Fine		0.5258 mol	0.5478 mol	4.19%

After the performance of the model was assessed, the parametric study was started. Four hundred permutations of H and C<sub>Ag+c</sub> were completed in the parametric study. The combination that provided the best silver ion release between

the 200 ppb and 400 ppb limit had the values of 0.0015 and 100 mol/m<sup>3</sup> for H and C<sub>Ag+,c</sub>, respectively. Therefore, the C<sub>Ag+,c</sub> of 100 mol/m<sup>3</sup> was selected for the experiment (this is the initial concentration charged in the sample chamber).

Gravity and its absence did not have any effects on the computer simulation. Figure 8 shows the silver ion output concentration from the dialyzer computer model and the three 8-hour experimental test runs. As can be seen from the data, the model predicted a transient spike at the start of the flow, up to 3000 ppb, a fairly rapid decrease over 50 minutes to a minimum output of 200 ppb, a short-lived increase in silver ion concentration over an approximate 40 minute period to a predicted silver ion release at about 300 ppb over the remainder of 8-hour simulation. A few of the modeled trends in silver ion release can also be observed in the experimental test runs. Like the modeled data, the first feature is a high concentration spike at the start of testing. Like the modeled data, the experimental data concentration is observed to drop to a minimum value thereafter. However, the decrease following the spike was more rapid for the experimental test runs, occurring over 12 minutes. Like the model, the silver concentration is then observed to increase following the minimum, but at a more gradual and long-lived rate. The release from experiment #1 was inconsistent with the expected behavior, and the results suggest that the membrane system requires preconditioning to perform as desired. Experiment #2 stayed the longest in the desired concentration range of all three experiments. For the three experimental runs, only in Experiment #3 was the silver ion concentration observed to level out around hour 6. The silver concentration was observed for the other two experimental runs to continue rising over the entire test run. The increasing release seemed between 2.5 hours and 7 hours for experiment #2 had an average release rate of 76.25 ppb/hr. In experiment #3, this increasing release occurred between 2 hours and 6 hours, resulting in an average release rate of 200 ppb/hr. While the experimental runs and first modeling attempt did not reproduce each other, they do show that a discrete release of silver ions can be achieved in the target range over the long term. Nevertheless, the silver ion release could be easily adjusted to the target range of 400 to 200 ppb by including a bypass to dilute treated water. More work will need to be done better to understand both the physical and modeled systems' behavior.



**Figure 8. Silver Ion Release by Dialysis-based Passive Biocide Delivery System.** The plot shows the dialyzer's outflow silver ion concentration during 8 hours from the experiments and that from the computer model. The dialyzer's sample chamber was loaded with a 100 mol/m<sup>3</sup> silver solution, and deionized water was supplied at 100 mL/min flow rate.

The experimental results also showed that the silver ion release increased with each successive experimental run. Experimental test #2 had higher output than experimental test #1, and experimental test #3 had a higher output than experimental test #2. The results may indicate that the membrane's pore size enlarges as the membrane is reused or membrane wetting is induced. This performance outcome was previously contemplated since dialysis is typically done with a single-use disposable device. Because of the preliminary nature of this study, only one dialyzer was tested. Thus, more experiments are required to validate the performance of this dialyzer. Ultimately, experiments should be run after keeping the dialyzer charged with the concentrated solution during dormancy.

Furthermore, the silver ion release data suggested that the selected MWCO may provide the desired pore size. The next commercially available MWCO is 3.5 - 5 kilo-Daltons, which is assumed to be too large for this application after preliminarily documenting the performance of the 0.1-0.5 kilo-Daltons MWCO. Polymeric membranes with an MWCO smaller than 0.1 - 0.5 kilo-Daltons will be acquired and tested.

## V. Conclusion

The preliminary study of the dialysis-based PBDS for spacecraft or extraterrestrial bases WRS was carried out by modeling the device, using COMSOL Multiphysics®, and testing an available dialyzer. The proposed dialysis-based PBDS device was computationally modeled to understand the silver ion release. The computer simulation results showed that the dialysis-based PBDS could sufficiently deliver silver ions to a stream of DI water for 8 hours. The computer simulation also revealed that the dialysis system would generate a highly concentrated spike when the process is initialized, and the silver ion release would not reach target levels until 50 minutes have passed. Nevertheless, the initial spike observed in the experiments reached the target levels earlier than predicted. Experimental test # 2 gave the longest silver ion release in the desired concentration range. The silver ion release from experimental test #3 is the data that best matches the model; however, the observed concentration is significantly higher than predicted. More extended experiments will be run to determine when the system starts delivering silver ions at a stable level as predicted. Moreover, the results showed that the dialysis membrane's reuse increases the silver ion output up to 40% after each run. More experiments are needed to validate the former statement statically. Even though the computer simulation results did not perfectly match those from the experiments, they provided a starting point to determine the initial  $C_{Ag+,c}$  of 100 mol/m<sup>3</sup> without including the effects of the counter ion and suggest a range of permeability needed to provide the desired release. Future work will modify the permeability model so that the simulation can match the experimental results. An accurate computer model would reduce the need for long experiments, large volumes of DI water, and extensive disposal of silver-containing water. Subsequent studies will continue investigating more reproducible and predictable silver ion release from the dialysis-based PBDS. Through this additional study, the testing of new organic and inorganic dialysis membranes and different silver salt solutions will be attempted. Future experiments will implement a silver ion-selective electrode for better experimental data acquisition. Ultimately, a process control strategy that can maintain the delivery system operating in a passive mode would need to be developed if a discrete steady-state release cannot be obtained from the dialysis system.

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