

Numerical Investigation of Heat Transfer and Fluid Flow within Electrochemical Hydrogen Peroxide Generation Unit

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Long-term manned space missions require the onboard production of disinfectants essential for maintaining crew health and supporting life systems. Currently, disinfection aboard the International Space Station (ISS) relies on disposable wetted wipes, which are regularly resupplied from Earth. This approach imposes a significant burden on resupply logistics, storage, and waste management. To address these challenges and support future missions, efforts are underway to develop an in-situ solution that electrochemically generates hydrogen peroxide disinfectant using onboard resources. The Peroxide Generation Unit (PGU) can produce up to 3 wt.% hydrogen peroxide on-demand at a rate of 1 liter per day, providing a sustainable alternative to Earth-dependent supplies. The resulting aqueous hydrogen peroxide (H_2O_2) is an effective disinfectant, safe for crew use, compatible with spacecraft systems, and free from volatiles, off-gassing, or residues. Generating hydrogen peroxide at the required rate needs high voltages and currents, exceeding 20V and 2A respectively, which leads to significant heat generation from Joule heating. This temperature rise poses a risk to sensitive system components, especially critical and expensive membranes that can degrade under thermal stress. In order to develop and assess risk mitigation strategies, the thermal, fluid, and electrical flows within the system are modeled computationally using the commercial software COMSOL. The numerical simulations are validated against experimental data from an alpha-scale system designed at Faraday Technology, Inc. Once verified, the model is employed to identify thermal hotspots, investigate their underlying causes, and explore solutions to prevent them.

Acronyms and Nomenclature

C_p	=	Specific heat capacity
CFD	=	Computational Fluid Dynamics
E	=	Electric field
H_2O_2	=	Hydrogen peroxide
h	=	Heat transfer coefficient
J	=	Current density

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k	= Thermal conductivity
μ	= Viscosity
P	= Pressure
q	= Heat flux
Q_J	= Joule heating energy
ρ	= Density
σ	= Electrical conductivity
T	= Temperature
u	= Velocity
V	= Electric potential

I. Introduction

Hydrogen peroxide (H_2O_2) is widely used as a disinfectant, oxidizer, and industrial chemical due to its strong oxidative properties and environmentally benign decomposition into water and oxygen. In recent years, electrochemical generation of H_2O_2 has gained significant attention as a sustainable alternative to conventional production methods, particularly for applications in space-based life support systems and resource-limited environments.[1; 2] The electrochemical reduction of oxygen to H_2O_2 offers a clean, energy-efficient route that eliminates the need for chemical precursors and minimizes waste.[3]

For long-duration space missions, in-situ generation of hydrogen peroxide is critical for ensuring crew safety and spacecraft hygiene while reducing logistical burdens. Currently, disinfectants used aboard spacecraft, such as pre-packaged hydrogen peroxide wipes or chemical cartridges, require periodic resupply from Earth, adding significant mass and storage constraints.[4] Additionally, these disposable wipes contribute to solid waste accumulation, which poses challenges for waste management in closed-loop space habitats.[5] Electrochemical synthesis of H_2O_2 directly from onboard resources—oxygen and water—offers a promising solution, enabling on-demand production of a disinfecting agent that can be applied to reusable wipes. This approach eliminates the need for single-use disinfectant wipes, thereby reducing both the carried and disposed waste associated with surface sterilization. Furthermore, H_2O_2 has potential applications beyond surface cleaning, including water purification, biofouling prevention in heat exchangers, and even medical sterilization.[6]

Additionally, hydrogen peroxide plays a crucial role in hydroponic systems for space-based agriculture. Maintaining microbial control within nutrient delivery systems is essential for plant health and food safety. Recent studies have demonstrated the effectiveness of H_2O_2 -based sanitization in hydroponic environments, preventing biofilm formation and ensuring the sustainability of sequential crop cycles.[7] Implementing an electrochemical peroxide generation system can enhance the reliability of spacecraft hydroponics while minimizing reliance on resupply missions from Earth.

Faraday Technology, Inc., in collaboration with NASA, has advanced the concept through a series of Small Business Innovation Research (SBIR) projects, resulting in the development of a Peroxide Generation Unit (PGU). The PGU can produce up to 3 wt.% hydrogen peroxide on-demand at a rate of 1 liter per day. The conceptual schematic of the system along with the electrochemical reactions at the anode and cathode are shown in Figure 1.[8; 9] Initial experimental studies have shown promising results, but also revealed the necessity of high voltages and currents, exceeding 20V and 2A respectively, to achieve the requisite peroxide generation rate. This results in significant heat generation due to Joule heating, and the subsequent temperature rise poses a risk to sensitive system components, especially critical and expensive membranes that can degrade under thermal stress.

Modeling the electrochemical H_2O_2 generation process is crucial for optimizing system performance, improving efficiency, and mitigating operational challenges such as membrane degradation.[10] This study aims to develop a comprehensive computational model that integrates thermal, fluid, and charge transport phenomena within an electrochemical peroxide generation cell. Understanding these coupled interactions is critical for predicting system behavior, optimizing operating conditions, and ultimately improving the longevity and stability of the system. A key motivation for this work is the observed membrane failures in existing systems, which limit operational lifetimes and impact overall efficiency.[11]

The initial modeling efforts will focus on simulating the heat transfer, fluid and electric current flow through the system. These factors play a significant role in determining reaction rates, ion transport efficiency, and temperature distribution across the system.[12] By establishing a robust model for these interactions, we will provide a foundation for incorporating electrochemical reactions with charge and mass transfer effects in future studies, enabling a more detailed investigation into membrane degradation mechanisms. Specifically, we aim to identify the role of local heating,

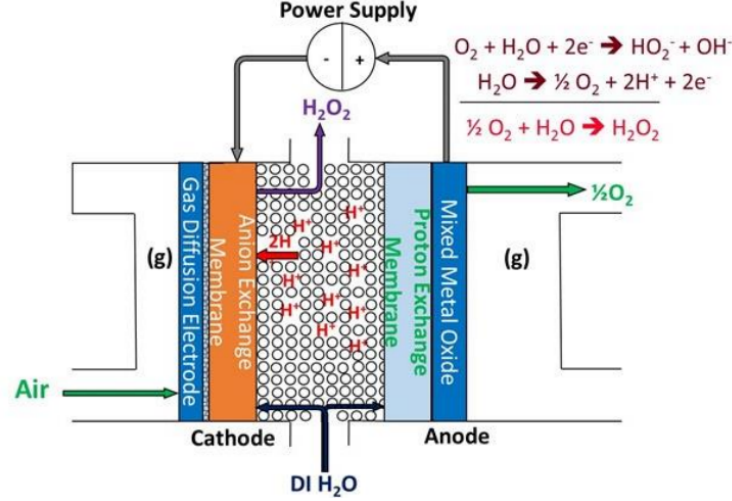


Figure 1. Conceptual schematic of the Peroxide generation units with single-cell chemistry.[9]

concentration polarization, and electrochemical stress on membrane stability, which are critical to improving reactor durability and ensuring sustained peroxide production.[13]

This work will contribute to the broader understanding of electrochemical H_2O_2 generation, providing insights into the fundamental transport phenomena governing system performance. By leveraging computational modeling and experimental validation, we seek to develop design strategies that enhance system reliability and efficiency, with applications ranging from space-based disinfection to terrestrial water treatment and industrial oxidation processes.[14]

II. Simulation Methodology

The primary source of heat generation in the system is Joule heating, which occurs due to the flow of electric current through the system. Since this work focuses on modeling the temperature within the peroxide generation unit, the electrochemical reactions are not explicitly modeled. The electrochemical reactions are assumed to operate at 50% efficiency, with the remaining energy dissipated as heat through Joule heating. This efficiency value is determined by comparing the experimentally measured peroxide yield to the theoretical yield predicted by Faraday's law. To account for this efficiency in our model, the voltage is scaled down by a factor of two.

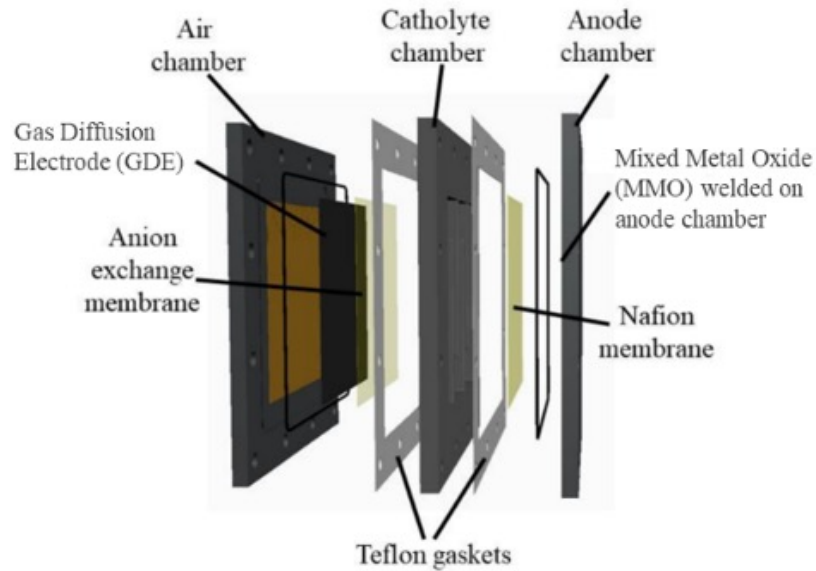
A. Geometry and Computational Domain

The schematic of the alpha-scale PGU setup, including all components, is presented in Figure 2, and the CAD model of the cathode, anode, and catholyte chamber is shown in Figure 3. The cathode plate is composed of gold-plated stainless steel (SS316) and features a central $5'' \times 5''$ flow field that facilitates airflow into the system. The anode plate consists of a titanium block with a mixed metal oxide (MMO) curved region at the center. The catholyte chamber, fabricated from PVC, incorporates a serpentine flow path. Two membranes separate the central regions of the catholyte chamber from the anode and cathode: Nafion for the anode side and Sustainion for the cathode side. Teflon gaskets are positioned between the chambers enclosing the central regions, to ensure that electrical current is conducted exclusively via ionic transport through the membranes. The entire assembly is secured using nuts, bolts, and washers. The material properties of the various components in this system are listed in Table 1.

The creation of the computational mesh of the MMO region in the anode proved particularly challenging due to its complex curvature. The final mesh, consisting of 250,000 vertices and 1.4 million elements, was computationally intractable. Given that the primary function of this central curved region is to ensure uniform airflow distribution across the central flow field, the cathode chamber design was adopted for the anode to facilitate the modeling process.

Table 1. Material properties used within the current numerical simulations.

Component	Material	Density (kg/m ³)	Heat Capacity (J/kgK)	Thermal conductivity (W/mK)	Electrical conductivity (S/m)
Cathode	Stainless steel SS316	8000	500	16.2	3.77×10^6
Anode	Titanium	4510	5230	17	1.8×10^6
Catholyte chamber	PVC	1320	1340	0.25	0.2
Anode membrane	Nafion	1980	1300	0.3	10
Cathode membrane	Sustainion	1100	1350	0.25	200
Gasket	Teflon	2200	1400	0.2	1×10^{-23}

**Figure 2. Schematic of the alpha-scale peroxide generation unit with the various components.[8]**

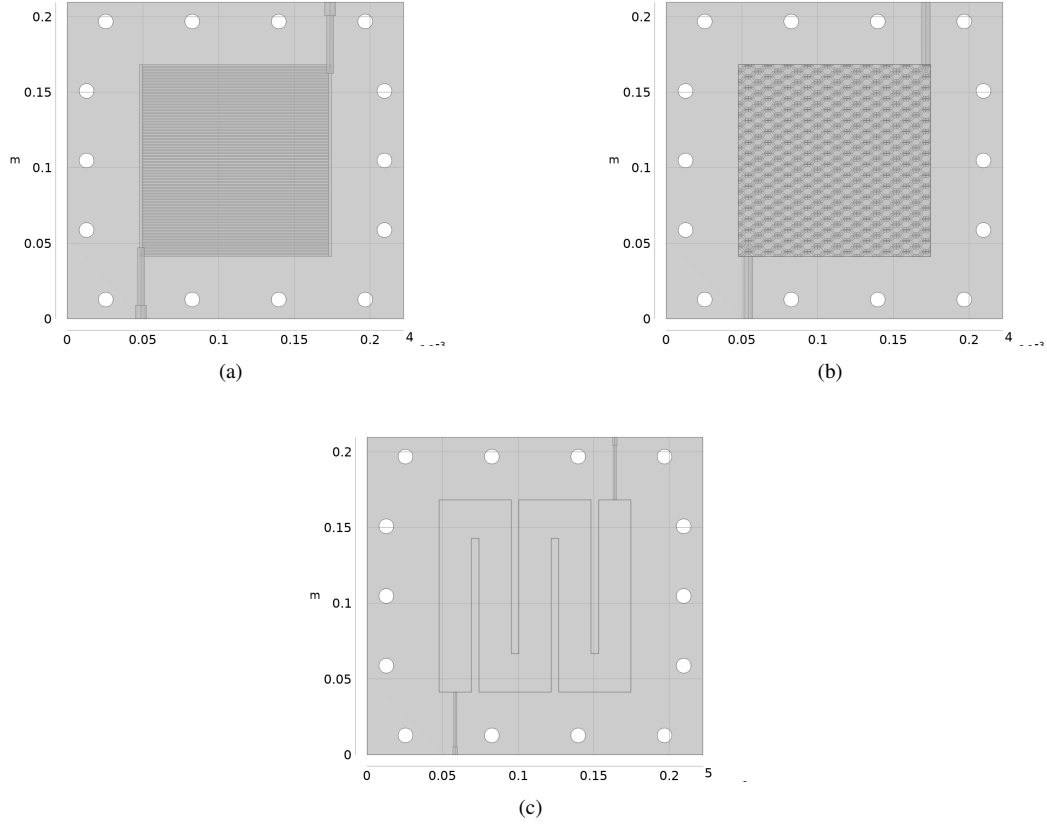


Figure 3. Computational domain of (a) cathode plate, (b) anode plate, and (c) catholyte chamber created within COMSOL.[15]

B. Governing Equations

The heat transfer, fluid and electric current flow through the system is solved at steady state. The governing equation for the stationary flow of current through the system is given by

$$\nabla \cdot \mathbf{J} = 0, \quad (1)$$

where ∇ is the gradient/divergence and $\mathbf{J}$ is the current density that is defined as

$$\mathbf{J} = \sigma \mathbf{E}. \quad (2)$$

$\mathbf{E}$ is the electric field and σ is the electrical conductivity. The electric field can be obtained from the electric potential V using

$$\mathbf{E} = -\nabla V \quad (3)$$

The heat losses occurring as a result of electric current flow through the system is described by the Joule heating term.

$$Q_J = \mathbf{J} \cdot \mathbf{E} \quad (4)$$

This is present as a source term within the heat transfer equations in both solids and liquids. For solids, this is expressed as

$$\nabla \cdot \mathbf{q} = Q_J \quad (5)$$

q is the heat flux in the system and is linked to the temperature T based on Fourier's law:

$$q = -k\nabla T. \quad (6)$$

k is the thermal conductivity of the system. For fluids, the Joule heating term is present in the energy equation

$$\nabla \cdot (\rho u C_p T) + \nabla \cdot q = Q_J \quad (7)$$

This energy equation is solved along with the steady-state continuity and momentum (Navier-Stokes) equations to obtain the final solution.

$$\nabla \cdot (\rho u) = 0 \quad (8)$$

$$\nabla \cdot (\rho u u) = -\nabla P + \nabla \cdot (\mu \nabla u) \quad (9)$$

The flow and heat transfer equations for the fluids are coupled by the velocity term in the energy equation, as well as the density term (which is a function of temperature) in the continuity and momentum equations. As discussed previously, the coupling between the electric current flow and heat transfer equations is provided by the Joule heating term.

C. Boundary Conditions

The system consists of three inlets: two for airflow, located in the cathode and anode plates, and one for water inflow in the catholyte chamber (Figure 4). The flow rate is specified at each inlet, with the assumption that the flow is fully developed within the tubing. At the three corresponding outlets, the pressure is set to an ambient pressure of 1 atm. Heat transfer from all external surfaces is modeled using surface-to-ambient radiation and natural convection. The ambient temperature was taken as 293 K and a standard heat transfer coefficient of 5 W/m²K was used. For electric current flow, the electrode locations are defined as applied voltage and ground. As previously mentioned, the electrochemical reactions consuming the electric current are not explicitly modeled. Instead, a reaction efficiency of 50% is assumed. Consequently, to account for the energy conversion losses, the applied voltage is reduced by half.

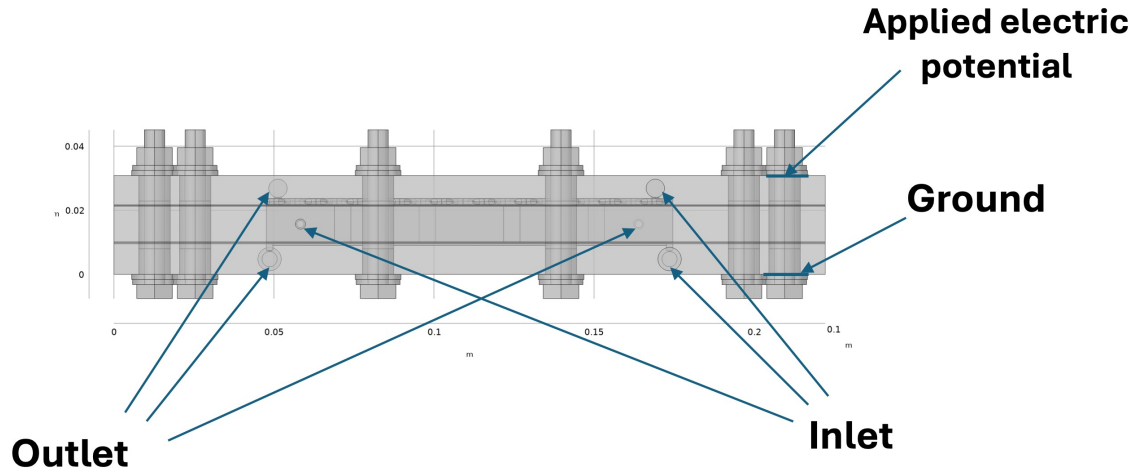


Figure 4. The final computational domain of the alpha-scale peroxide generation unit along with the boundary conditions.

D. Solution Procedure and Grid Independence

The CAD model of the various components and the final computational domain was created using the commercial software package COMSOL.[15] This domain was then discretized and meshed using tetrahedral elements. Multi-physics

simulations for heat transfer, fluid flow, and electric current flow were also performed within COMSOL. The Reynolds number at the narrowest region for the air (~ 200) and water (~ 1) flow was much lower than the turbulence threshold and therefore laminar flow model was employed in all the simulations. The finite volume method was employed to solve the coupled equations iteratively using the generalized minimum residual method (GMRes), with a convergence criterion set at $1e-6$. The fully coupled system of equations for the steady state system is solved within COMSOL using the PARDISO (PARallel DIrect SOLver) direct solver.[15]

A mesh-independence study was conducted by considering five different mesh configurations with 57,000, 130,000, 252,000, 506,000, and 1,007,000 cells, obtained by varying the element size for the same geometry. The study demonstrated that the simulations using the intermediate mesh with 252,000 cells yielded satisfactory numerical accuracy. Variations in global parameters, including fluid outlet temperature, average surface temperature, mass flow rate, and current density, were all within 1.5% relative to the finest mesh. Therefore, this mesh size was selected for all subsequent simulations.

III. Results and Discussion

Significant heat generation has been observed in the current PGU setup at Faraday Technology, Inc.[8] The generation of hydrogen peroxide at the required rate necessitates high voltages and currents, exceeding 20V and 2A, respectively. These conditions lead to elevated temperatures and rapid degradation of components, particularly the ion-exchange membranes. The primary objective of the present study is the thermal modeling of the PGU system and the identification of local hot spots within the system. To achieve this, the full geometric design of the system is incorporated into the computational model, as opposed to the simplified designs typically used in electrochemical simulations. However, as a tradeoff, the electrochemical reactions are not explicitly modeled, and their occurrence is assumed to be governed by a specified efficiency. This initial simplified model provides a detailed thermal map of the intricate system geometry and enables the analysis of the effects of design modifications. Future work will explore the incorporation of electrochemical reactions into the current system model.

A. Validation

First, the numerical simulation is validated against experimental data obtained from Faraday Technology, Inc.[8] The PGU system was configured to produce a 3 wt.% hydrogen peroxide solution with an applied voltage of 22 V. The total current in the system was measured to be 2.5 A. The air flow rate was set to 100 mL/min, while the water flow rate was 20 mL/min. The inlet air temperature was approximately 293 K (20°C), typical of ambient room conditions, while the water was pre-chilled to 278 K (5°C) before being introduced into the catholyte chamber. For the numerical simulations in COMSOL, all experimental parameters were maintained, except for the input voltage, which was halved to 11 V due to the electrochemical reactions not being explicitly modeled and the assumed efficiency of 50%. This efficiency value is calculated using the ratio of the experimental peroxide generation to the amount of theoretical peroxide generation calculated by Faraday's law. A thermocouple was placed at the center of the top side of the anode block, where the measured temperature was around 300 K (27°C). In the simulation, the average temperature at the same location was observed to be around 298 K, which shows good agreement with the experimental data. This close match instills confidence in the numerical approach used in this work. Currently, efforts are underway to set up the PGU system at NASA Johnson Space Center, with plans for more detailed temperature measurements and further validation of the numerical simulations.

B. Analysis

The temperature and flow velocity distributions within the cathode, anode, and catholyte chamber are analyzed to gain a deeper understanding of the PGU system. Each of these components consists of an outer solid region and an inner fluid region. Figure 5 illustrates the temperature contour plots for both the outer and inner regions, as well as the velocity map for the inner region. The maximum temperature in the outer region is approximately 312 K, occurring in the top-right corner near the electrode location. A similar heat distribution is observed within the inner fluid region, where the highest temperature, around 305 K, is also found in the top-right corner. The velocity profile indicates that the air slows down as it enters the central chamber. We also notice that the air is evenly distributed throughout the chamber due to the groove channels, which would be beneficial for electrochemical reactions by increasing the effective surface area.

Figure 6 shows the same plots for the anode. Similar temperature and velocity profiles are observed. The maximum temperature in the inner region is approximately 307 K, while in the outer fluid region, it is around 317 K, which is the

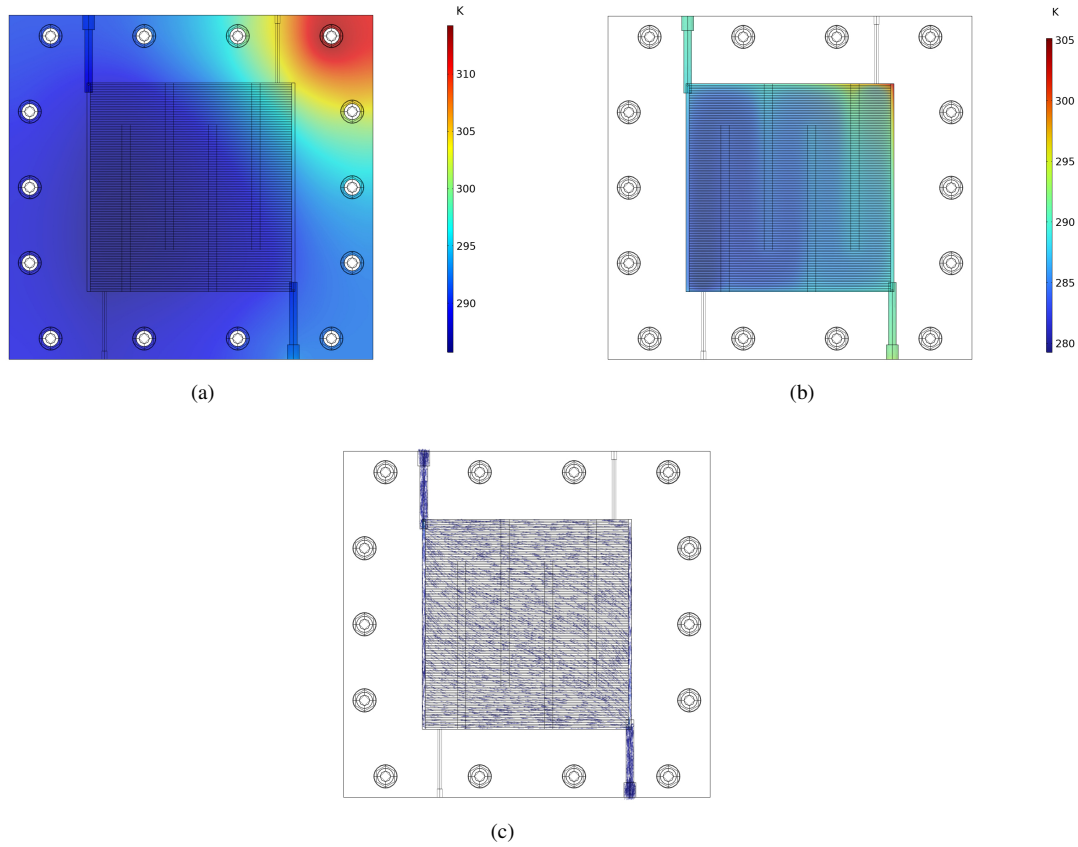


Figure 5. Temperature contour plot of (a) the outer solid region, and (b) the inner fluid region, and (c) Velocity arrow map in the inner fluid region of the cathode.

overall maximum temperatures within the system.

The temperature and velocity profiles for the catholyte chamber are shown in Figure 7. The heat distribution is quite similar to that observed for the anode and cathode, with the maximum temperature occurring in the top-right corner. The maximum temperature in the outer and inner regions is 315 K and 306 K, respectively. The temperature within the catholyte chamber is lower than that in the anode but higher than in the cathode. The velocity profile, however, differs significantly from the previous cases since the fluid is water instead of air. The flow tube expands rapidly into the central chamber, causing the water to decelerate considerably. This reduction in velocity is further amplified by the serpentine path in the central region, which also facilitates the electrochemical process.

C. Effect of Electrode location

The peak in the temperature map of the current system design occurs near the electrode locations. While this is expected, the temperature rise is further exacerbated by the presence of both electrodes being mounted on the same bolt. To reduce the system temperature, a modification is proposed in which the electrodes are attached to diametrically opposite bolts. A numerical simulation of the modified design is performed to assess the effect of increasing the distance between the electrodes. The results of these simulations are presented in Figure 8 and compared with the original design. It is observed that although the hot spots still occur near the electrodes, the temperature distribution is more spread out due to the increased distance between the electrode locations. The maximum temperature is found to be around 313 K, which is 4 K lower than that of the original design. Therefore, the proposed design modification is effective in lowering the temperature and is highly recommended.

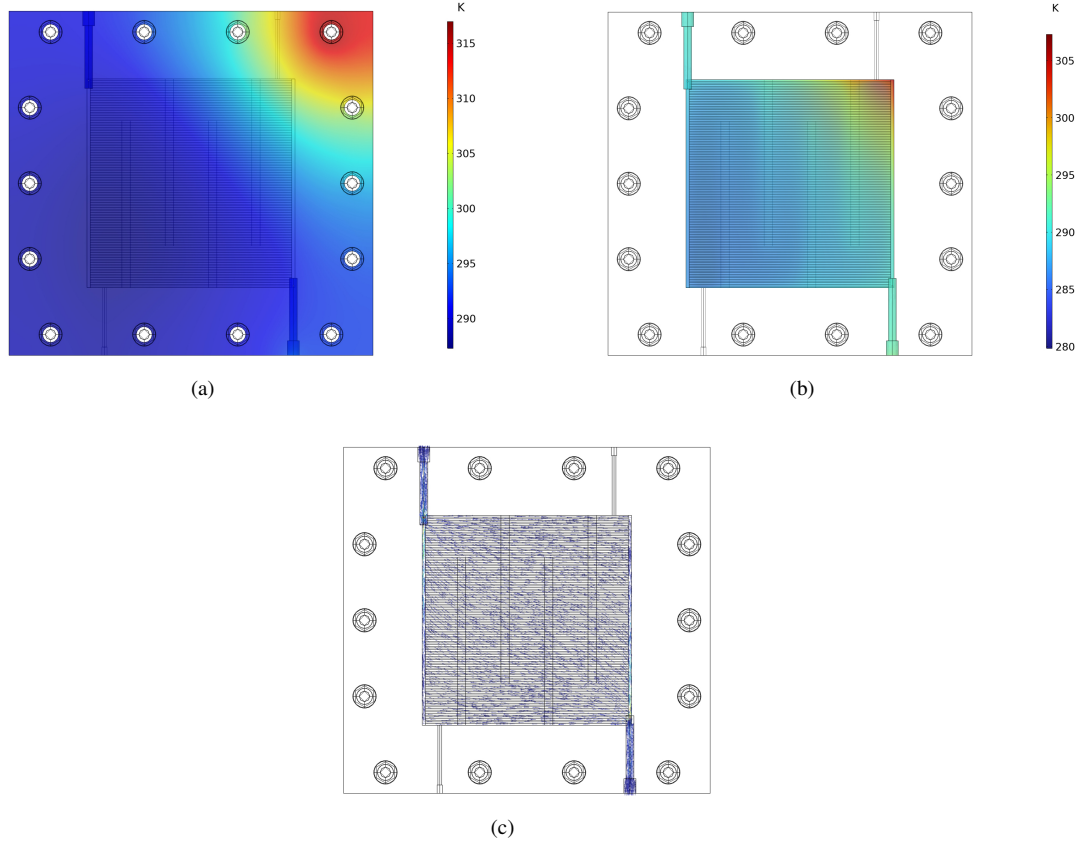


Figure 6. Temperature contour plot of (a) the outer solid region, and (b) the inner fluid region, and (c) Velocity arrow map in the inner fluid region of the anode.

D. Effect of Channels

The groove channels in the cathode are incorporated into the system to efficiently distribute air throughout the entire central region. This section investigates the effect of these groove channels on the temperature and velocity of the airflow within the cathode. A new cathode CAD model is created without the grooves, featuring an empty central region. Numerical simulations are conducted with this modified cathode design and compared to the original, as shown in Figure 9. It is evident that in the case without the grooves, the airflow is directed diagonally between the inlet and outlet tubes. The air density away from the direct path between the inlet and outlet is relatively low, which reduces the heat dissipation efficiency of the airflow, as reflected in the temperature map. This is particularly critical for the current design, where the peak temperature occurs outside the air flow region in the absence of the grooves. The case without the grooves shows a maximum temperature of 309 K, which is 2 K higher than the maximum temperature in the original design with grooves. Additionally, the absence of grooves reduces the effective surface area for electrochemical diffusion and reactions.

E. Effect of Water Inlet Temperature

A parametric study is conducted to evaluate the effect of water inlet temperature, water flow rate, and air inlet temperature on the thermal map of the PGU system. Figure 10 (a) shows the overall maximum temperature, as well as the temperatures of the Sustainion and Nafion membranes as a function of the water inlet temperature. The membrane temperatures are plotted, as they are critical for the sustained operation of the system over long durations. Five different water inlet temperatures are considered: 274 K, 278 K, 283 K, 288 K, and 293 K (1°C, 5°C, 10°C, 15°C, and 20°C). In this study, the water and air flow rates are kept constant at 20 mL/min and 100 mL/min, respectively.

All three temperatures are observed to increase significantly with the water inlet temperature, particularly the membrane temperatures. This is expected, as the water is in direct contact with both membranes. The temperature

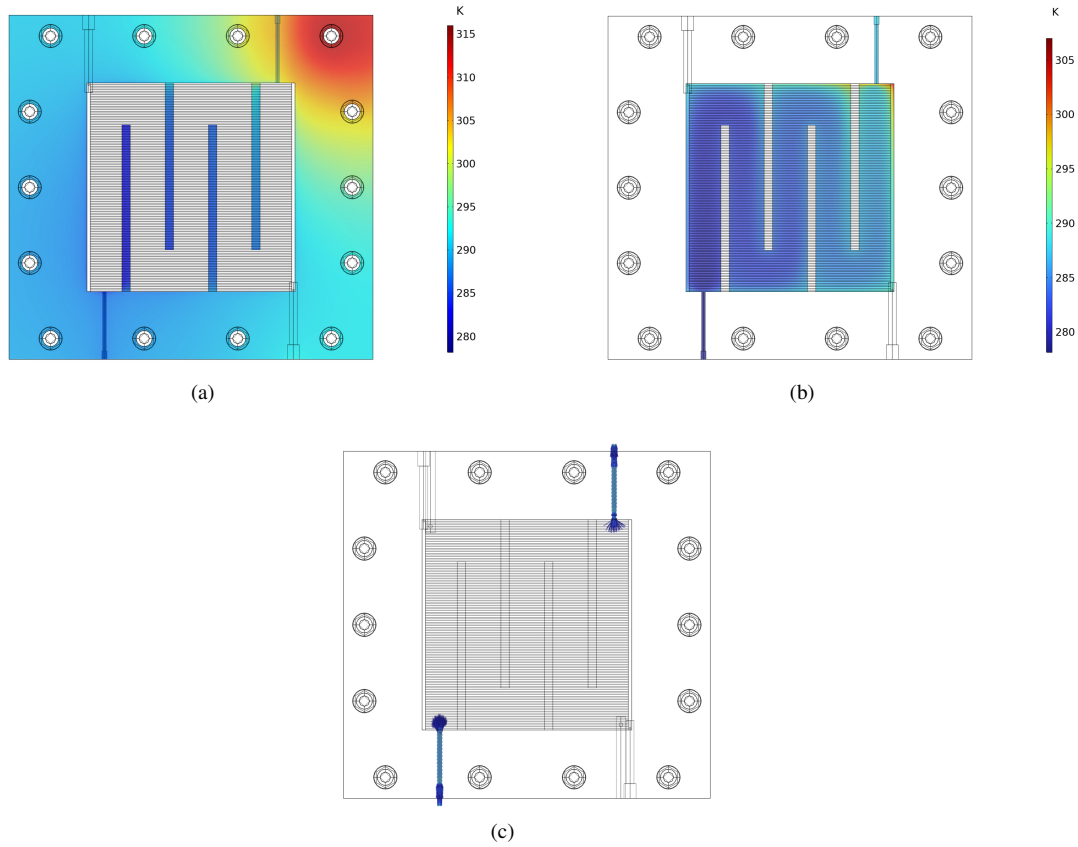


Figure 7. Temperature contour plot of (a) the outer solid region, and (b) the inner fluid region, and (c) Velocity arrow map in the inner fluid region of the catholyte chamber.

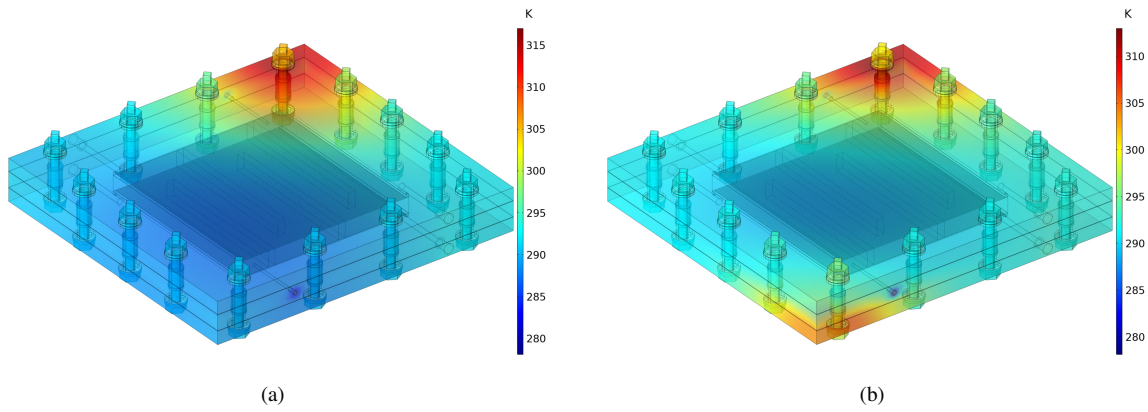


Figure 8. Temperature contour plots of the (a) current and (b) modified PGU system design.

variation is found to be linear, with a 13 K difference in the membrane temperatures between the two extreme water inlet temperatures considered. Thus, adjusting the water inlet temperature is a highly effective means of reducing the membrane temperatures.

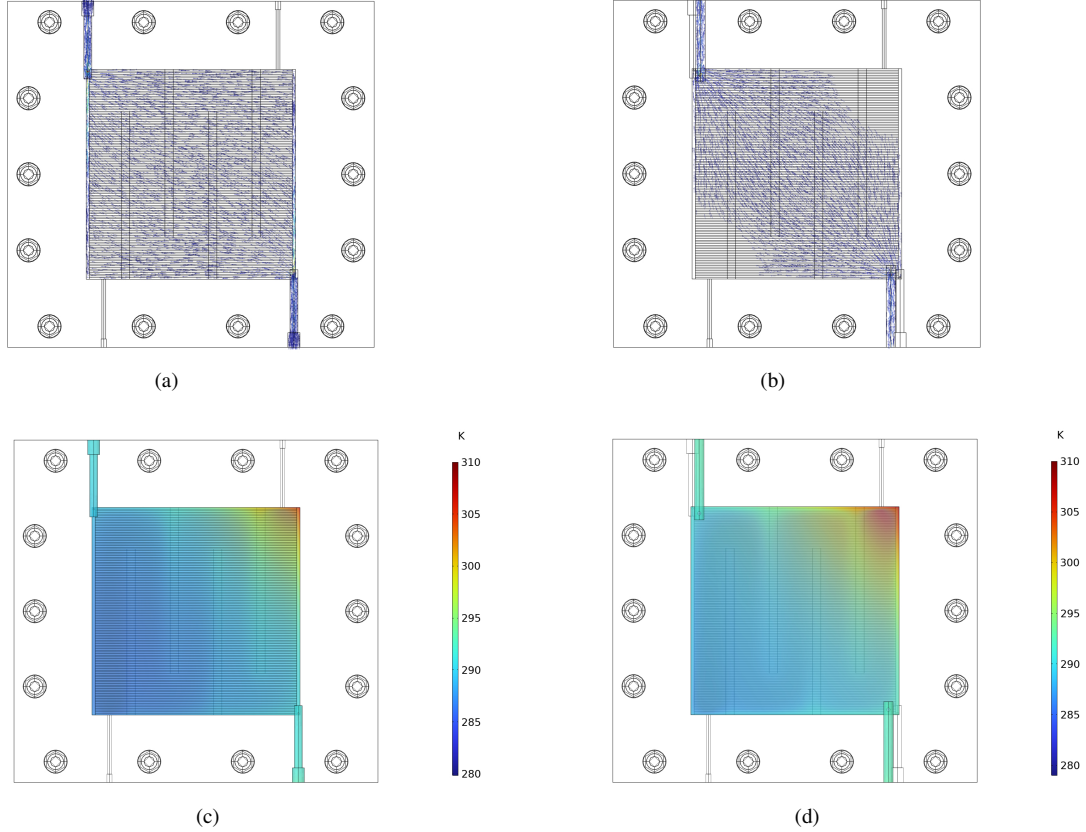


Figure 9. Velocity arrow maps within the cathode inner region (a) with and (b) without grooves. Temperature contour plots within the cathode inner region (c) with and (d) without grooves.

F. Effect of Water Flow Rate

Next, the effect of water flow rate on the system temperature is investigated. Figure 10 (b) shows the overall maximum temperature, as well as the Sustainion and Nafion membrane temperatures as a function of the water flow rate. Five different water flow rates are studied: 10 mL/min, 15 mL/min, 20 mL/min, 25 mL/min, and 30 mL/min. The water inlet temperature is kept constant at 278 K (5°C), and the air flow rate is set at 100 mL/min.

All three temperatures are found to decrease as the water flow rate increases. This is consistent with expectations, as water has a high specific heat capacity and can absorb a significant amount of heat from the system. The higher the water flow rate, the greater the heat dissipation, leading to lower temperatures. The temperature variation can be well-fitted to a power law expression with a small negative exponent (not shown), indicating diminishing returns with increasing water flow rates. There is only a 4 K difference in the membrane temperatures between the 10 mL/min and 30 mL/min water flow rates, suggesting that this is not as effective as the water inlet temperature in controlling the system temperature. Although the pressure drop across the system exhibited considerable variation with flow rate, all values remained relatively low (on the order of 100 Pa) and are therefore not considered to be of practical significance.

It is also noted that there is a significant variation in the pressure drop across the system at the different flow rates considered here. However all the values of the pressure drop

G. Effect of Air Flow Rate

Finally, the effect of the air flow rate on the temperature distribution of the system is studied. Figure 10 (c) shows the overall maximum temperature, as well as the Sustainion and Nafion membrane temperatures as a function of the air flow rate. Similar to the previous studies, the other two parameters: 293 K (20°C) water inlet temperature and 20 mL/min water flow rate, are kept constant. Five different air flow rates are considered: 50 mL/min, 75 mL/min, 100 mL/min, 125 mL/min, and 150 mL/min.

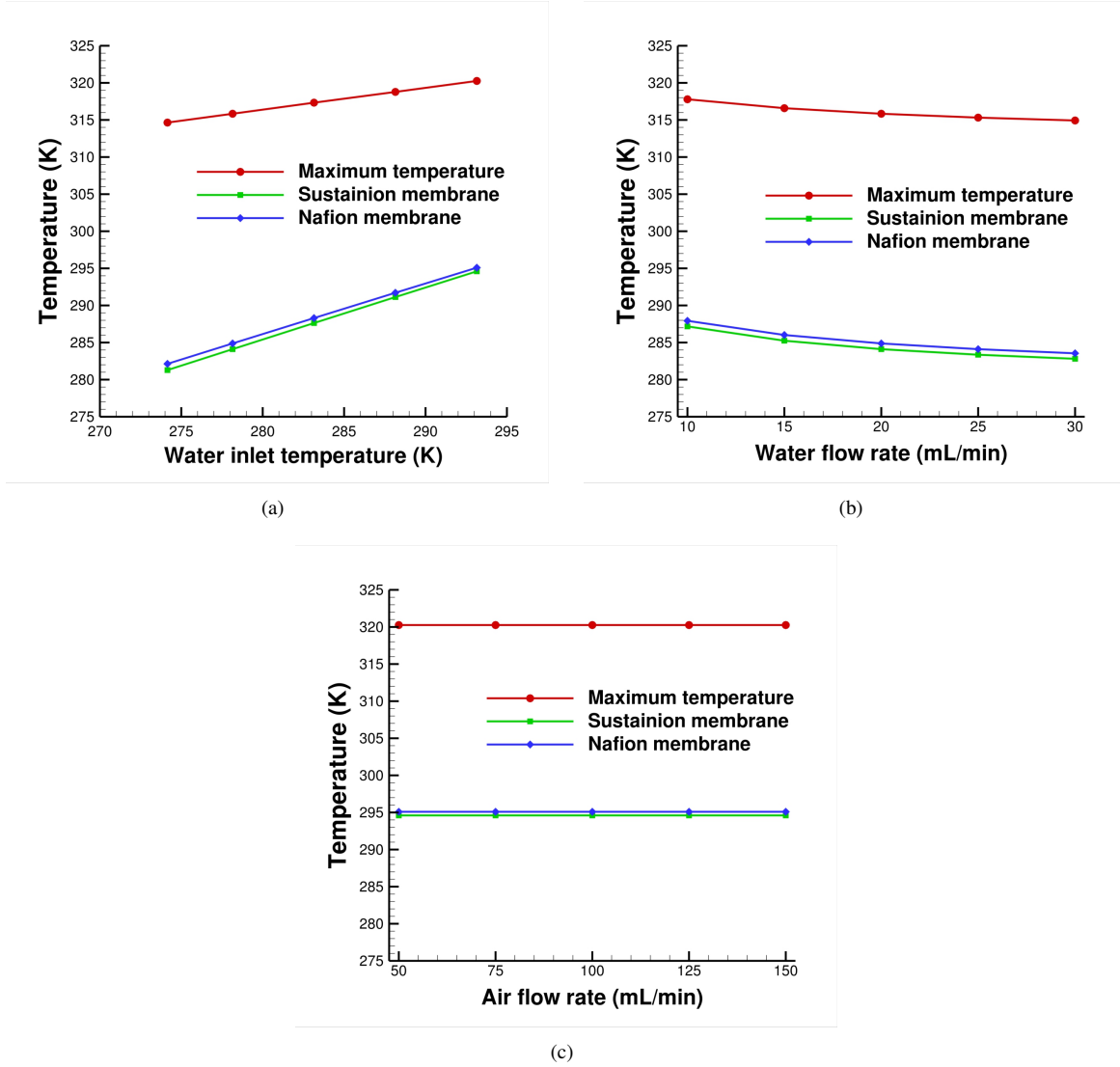


Figure 10. Variation of maximum, sustainion membrane, and nafion membrane temperature as a function of (a) water inlet temperature, (b) water flow rate, and (c) air flow rate.

It is observed that there is no significant change in any of the temperatures as the air flow rate increases. Although air is in contact with both membranes, similar to water, it does not play a major role in heat dissipation with the current design. Therefore, it cannot be used as a means to control the system's temperature.

IV. Conclusion

The fluid flow and temperature profile of the PGU system, designed to produce hydrogen peroxide for disinfection aboard the International Space Station (ISS), were investigated to identify thermal hotspots, understand their underlying causes, and explore potential solutions for mitigating them. The exact geometry of the system was incorporated into the numerical simulations, with the electrochemical reactions modeled simplistically using a single efficiency value. The study focused on the Joule heating resulting from the flow of electric current, its dissipation through the system, and the flow dynamics of both air and water. Numerical simulations were conducted using the multi-physics CFD solver COMSOL. A grid independence study was performed to determine the optimal mesh that provides both numerical accuracy and computational efficiency. This mesh size was then used to validate the system against temperature measurements of the PGU system from Faraday Technology, Inc.

A detailed analysis of the thermal map and velocity profile was conducted within the three primary components of the system: the cathode, anode, and catholyte chamber. It was found that the maximum temperature occurred at the

anode, near the electrode locations. Based on this analysis, a design modification was proposed in which the electrodes are positioned diametrically opposite, rather than being mounted on the same bolt. Numerical simulations of this modified design showed a significant temperature reduction of about 4 K. Furthermore, it was identified that the grooves in the cathode and anode play a crucial role in ensuring the uniform dissipation of air throughout the central region. This design feature contributes to an increase in both the heat dissipation efficiency and the effective contact area with the membrane, required for the electrochemical reactions.

Finally, a parametric study was conducted to assess the impact of water inlet temperature, water flow rate, and air flow rate on the overall maximum temperature and membrane temperatures. The study concluded that the system temperature was only affected by the water flow rate and inlet temperature, not by the air flow rate. The water flow rate had a minor, yet significant, effect on the system's thermal profile, with diminishing temperature reduction at higher flow rates. In contrast, the inlet water temperature had a substantial impact on system temperatures, exhibiting a linear dependence. This parameter was identified as the most effective for controlling the system's temperature.

V. Future Work

Once the experimental setup of the current alpha-scale PGU system is complete, more validation tests of the temperature profile will be performed. In addition, the next step is to include the modeling of electrochemical reactions in the system with the mass and charge transfer of ions and electrons. The goal of these future modeling efforts is to obtain the polarization curve[16] using COMSOL to assess cell efficiency and to perform Multi-Criteria Optimization Analysis using ASPEN.[12]

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