Modeling the impact of reaction-diffusion processes within a polyethylene glycol-based hydrogel coating in a microbial electrochemical cell

by

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Abstract

Microbial electrochemical cells (MECs) provide opportunities for energy production while treating wastewater. The environments these electroactive bacteria are exposed to are dynamic and can be difficult to emulate in a laboratory setting. This report demonstrates the feasibility of a model that simulates reaction-diffusion processes within a protective polyethylene glycol (PEG) - based coating over a bioanode operated as a Microbial Electrolysis Cell (a MEC) in a wastewater environment. The coating is designed to reduce the transport of undesired chemicals to the biofilm. COMSOL modeling software was used in conjunction with experimentally determined diffusion coefficients, reaction rates, and assumed boundary conditions to create two transient models of chemical concentration throughout the hydrogel. One of these models simulated the introduction of ammonia into the environment. The other model simulated the introduction of hydrogen peroxide into the system when the hydrogel was loaded with hydrogen peroxide degrading (catalase) enzymes. These models can be used to inform experimental conditions that are relevant to the design and development of these coatings. They can be adjusted to simulate the effect of factors such as toxin concentrations within bulk wastewater, the amount of enzyme loaded within the gel, and the reaction kinetics within the gel. With additional testing, this model can be used to optimize the hydrogel system to reduce the impact of toxins on biofilm activity while maintaining flow of nutrients to the microbes for metabolism and energy production.

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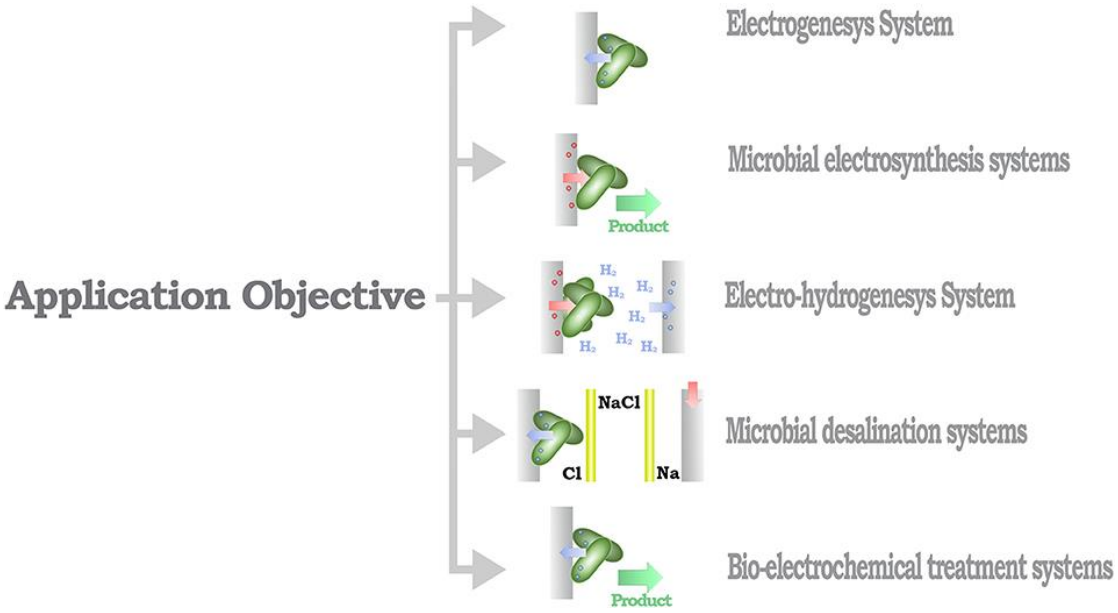
Introduction

Microbial electrochemical systems (MESs) provide an alternative approach to generating renewable energy with the potential to fill gaps in society's energy portfolio. In many cases MESs absorb and convert chemicals that are unsuitable for release into the environment, such as those found in wastewater. These wastewater systems expose the growing microbial biofilm anode cells to irregular environments, where there can be periods of limited nutrient availability and devastating spikes of environmental stressors. A polyethylene glycol (PEG) - based hydrogel is one method to reduce the microbe's exposure to these harmful spikes. This hydrogel is used to provide a protective layer for the cell's anode by limiting diffusion rate and providing opportunity for reactions to reduce concentration. The effectiveness of this hydrogel can be difficult to emulate in a laboratory setting for dynamic environments. The time and resources required for each test significantly limit the number of lab experiments that can be done. This report demonstrates the feasibility of using finite element software to model impactful chemicals that may be in the environment and their transient interaction within a PEG hydrogel coating. COMSOL modeling software was used to generate a transient model for ammonia diffusion as well as a model for hydrogen peroxide with a (catalase) enzyme loaded into the PEG coating. These models were created using diffusion coefficients, reaction rates, and assumed boundary conditions derived from preliminary experiments performed in the lab. By adjusting factors such as concentration in the bulk feed, the loaded amount of enzyme or other reactant, and reaction kinetics, this model can provide efficient feedback on both major and minor changes to the environment or hydrogel. This paper will additionally demonstrate how these changes are able to be modeled to provide insight into the significance of changing a given factor in the system.

Background

Microbial electrochemical systems use microbial biofilms that naturally develop on electrodes to generate energy. The potential for this interaction was first described in 1911 by English botanist Potter. However, this technology has only gained significant traction in the last 30 years.[1] In general, the microbial biofilm is coated on the system's anode, such as in microbial fuel cells (MFCs). However, MESs can be of "anodic (substrate oxidation) or cathodic (substrate reduction) nature."[1] The energy is harvested from the cells through electronic transfer as the cells use their basic enzymatic function.[2] These enzyme reactions use a variety of redox substrates which are exploited to generate electricity and/or other value-added products and can be classified into groups based on desired function. [3] Figure 1 below shows several MES classifications based on functionality driven parameters.

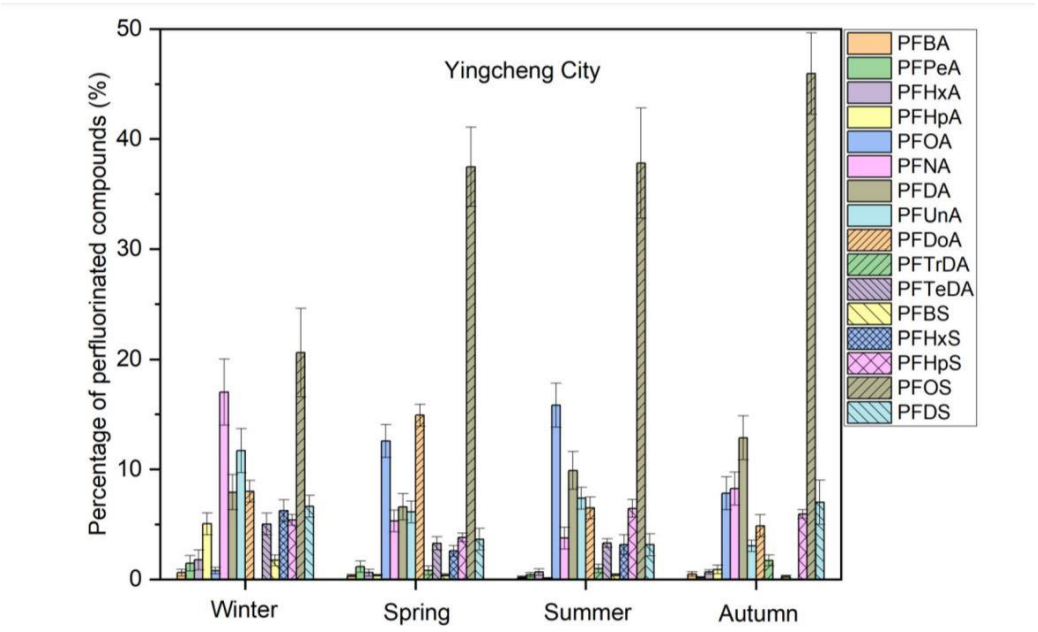
Figure 1. "Schematic organization of the MES classification based in the application objective and exemplary diagrams for each application"[1]



These systems require an interdisciplinary-minded approach, as the complexity of these systems requires understanding of factors such as electrochemical interactions, microbial physiology, and engineering principles so that the process is optimized to yield the most value-added results. [4] For example, it is not enough to just understand the electrochemical interactions for a microbe in the ideal environment but also to understand how they may interact with other microorganisms and change functions to defend against competition. Changes in these functions may impact the generation of energy, yield of other products, growth of the microbes, resource usage, and health of the system.[4]

The importance of this understanding is highlighted when considering the environments these systems are being explored for. Wastewater treatment, as an example of one of the fastest growing fields exploring MES technologies, demonstrates the importance of a multidisciplinary approach.[1] Figure 2 from Na et al. shows how perflourinated compounds varied in the waste sludge at a Yingcheng city wastewater treatment plant over the course of a year. Fluctuations like these are not specific to a single compound in the system.

Figure 2 Percentage of perluorinated compounds in the wastewater at a treatment plant in Yingcheng city[5]



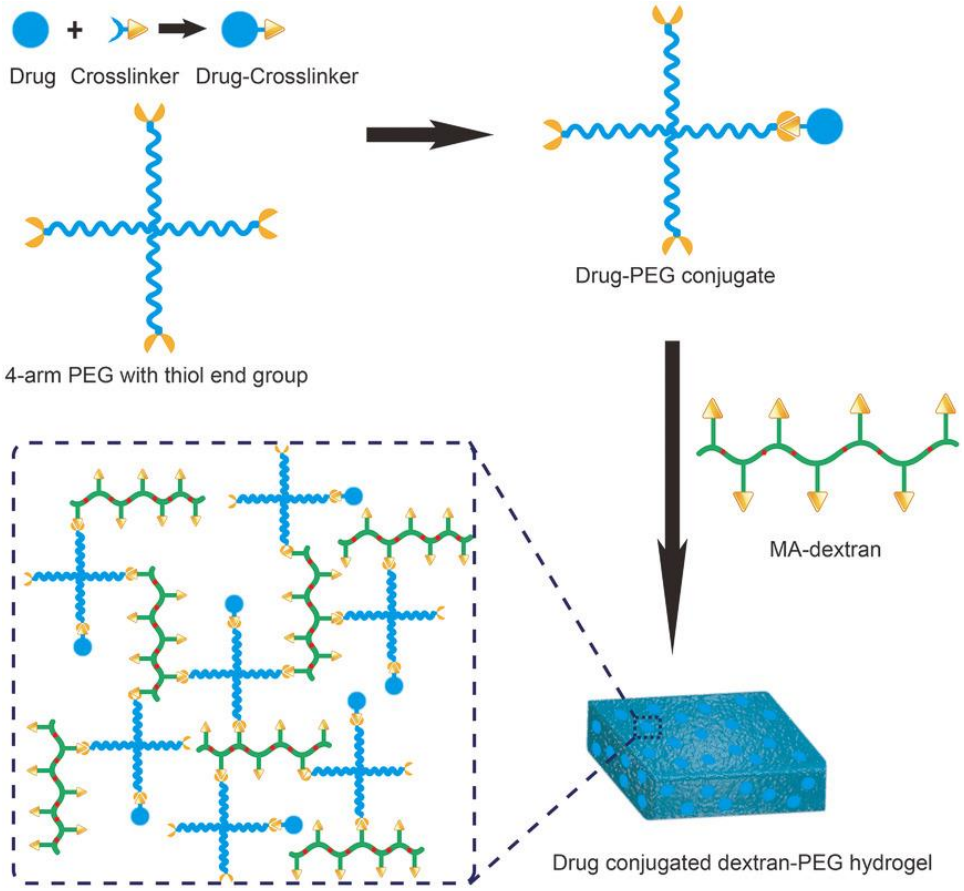
This magnitude of fluctuation is not specific to sewage wastewater. Environments such as seas and rivers are also dynamic and can be seasonally polluted by farm and industrial runoff. Runoffs can cause a spike in nutrients and stressors for systems and can also induce growth of undesirable microbes such as algae, potentially leading to algae blooms.[6] These can damage desired growth and slow the desired enzymatic reactions in the biofilm. Without an appropriate MES design configuration that limits the impact of environmental stressors while also optimizing the flow of nutrients to the biofilm, these systems cannot achieve the needed reliability and process efficiency for large scale implementation.

Hydrogels, such as PEG, provide an improved solution for reducing the impacts of dynamic environments on MES. PEG has been researched for many applications as it can be structurally adapted for different desired effects. For example, Lundberg et al. was able to generate several PEG coatings that were comprised of different structural blocks. In their

experiment, they determined that longer PEG chains improved their goal of antifouling performance.[7] This demonstrated one method of how the PEG properties can be easily adapted to fit a desired coating effect.

Wang et al. studied the use of PEG hydrogel with a dual function for treating wounds. The hydrogel in this case was loaded with antibiotics as seen in Figure 3. This crosslinked antibacterial was shown to be effective against *E. coli* and *S. aureus* and provides a way to avoid systemic side effects of the antibacterial as it is immobilized within the gel.[8]

Figure 3 Preparation of antibiotics conjugated dextran-PEG hydrogel.[8]



Along with acting as a treatment for bacterial contamination, this coating also served to keep a wound's environment more stable. These hydrogels also maintained moisture for the wound to accelerate healing by improving conditions for desired cell growth.[8] These factors can also be applied to protect the microbial biofilm in MESs by building catalysts and enzymes into the gel, effectively removing stressors while minimally impeding nutrient flow.

Despite the extent of research performed on the many MES factors, there is still a need for significant design improvements. In a laboratory setting optimized systems show notable potential for energy generation however, this technology does not live up to expectation when scaled and placed in a dynamic environment.[9] If feasible, the ability to model the variable environment and technical limits for microbial growth would remove some of the design barriers for these systems. This report will demonstrate how a simulated model can be effective for better understanding how a PEG coating will react when implemented in a laboratory or other dynamic environment.

Methodology

An initial steady state model in COMSOL of acetate diffusion and reaction for PEG around an MES was the base model for this work.[10] This defined the geometry and provided a comparison of experimental data from the laboratory to the simulated system in COMSOL. In this report, that model was extended to model the dynamic environment an MES would experience when in use.

Two simulated transient models were generated to test the feasibility of modeling MES systems with PEG coating. One to test the diffusion of ammonia that may spike in the surrounding environment and one to test the diffusion of hydrogen peroxide through a gel that was loaded with peroxidase, an enzyme that can react hydrogen peroxide to water and oxygen. For the ammonia model, the defined conditions are shown in Table 1. Additional information can be found in Appendix A.

Table 1 Conditions for ammonia diffusion-reaction model

Condition	Range
Concentration in bulk fluid	$800\ to\ 10000\ \frac{mg\ NH_3}{L_{H2O}}$
Diffusion Coefficient (Provided from experimental testing in the lab)	$1.75 * 10^{-6} to\ 2.225 * 10^{-6}\ \frac{cm^2}{s}$
PEG gel thickness (Provided from baseline model)	$700\ to\ 800\ \mu m$
Surface reaction rate (See Appendix A for more information)	$2.67 * 10^{-7} to\ 5 * 10^{-7}\ \frac{mol}{m^2 s}$

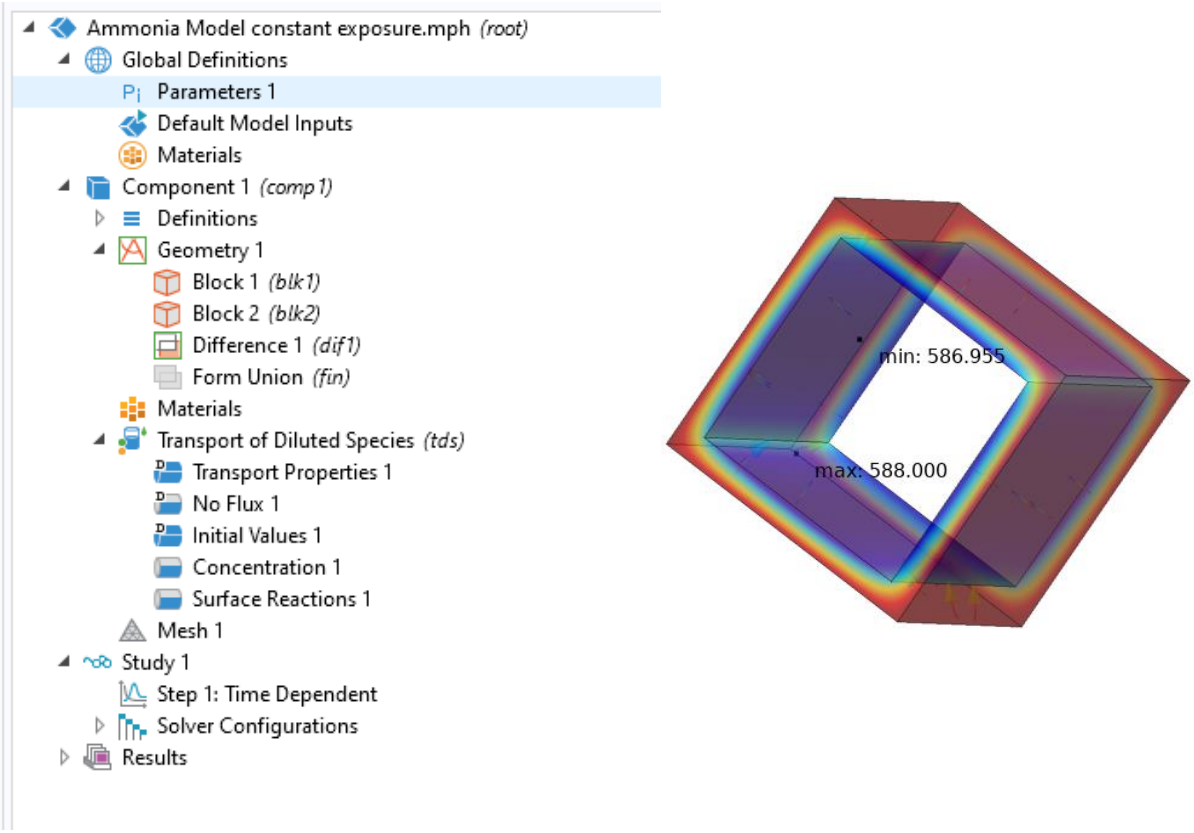
The hydrogen peroxide defined conditions can be seen in Table 2. Additional information can be found in Appendix B.

Table 2 Conditions for hydrogen peroxide diffusion-reaction model

Condition	Range
Concentration in bulk fluid	$47 – 588\ \frac{mol}{m^3}$ The concentration used may not accurately model wastewater and was used for demonstration of enzyme load
Diffusion Coefficient (See Appendix B for more information)	$1.32 * 10^{-6} to\ 1.68 * 10^{-6}\ \frac{cm^2}{s}$
PEG gel thickness (Provided from baseline model)	$700\ to\ 800\ \mu m$
Peroxidase reaction rate[11] Michaelis – Menten catalyst enzyme $E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \overset{k_3}{\rightarrow} E + P$ P in this case is H2O and O2	$k_1 = 10^4 \frac{m^3}{s * mol}$ $k_2 = 0.2 \frac{1}{s}$ $k_3 = 4.2 \frac{1}{s}$

Figure 5 shows the COMSOL sections that were set up for the transient ammonia model without events and an example of a steady state solution in 3D. The geometry is specified by two blocks. This allows for a 3D system with internal and external boundaries that fully represents the structure of the coating on the anode modeled.

Figure 4 Left basic COMSOL set up and right 3D example model of simulation



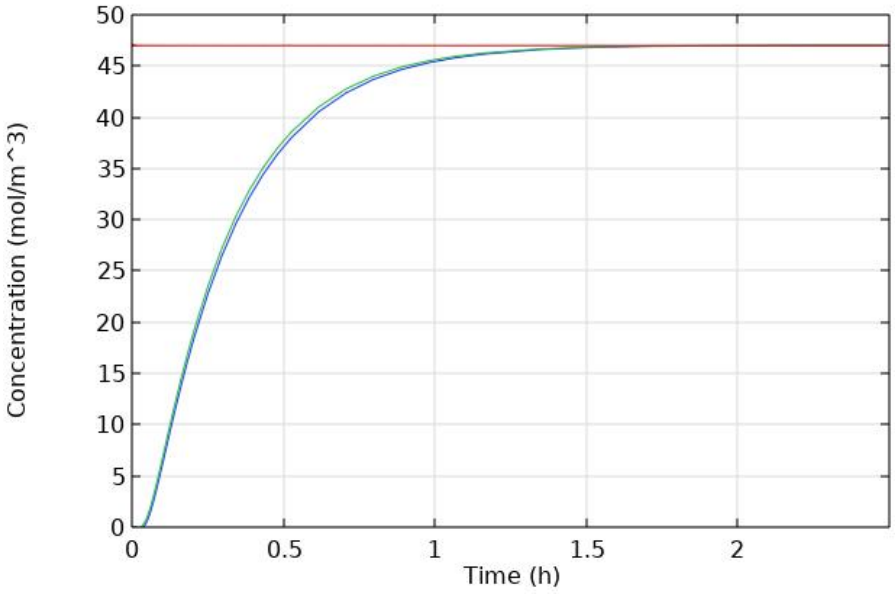
The "transport of dilute species" allows for all concentrations, flux, and simple reactions to be defined. An additional chemistry model is required for more complex reactions such as Michaelis – Menten. An example of this can be seen in Appendix C for the hydrogen peroxide model. The transient model can be run for a longer study time to determine steady state parameters that can be compared to laboratory experiments and used to confirm the base model's effectiveness before parameters are changed. The study defines the length of time of the model and what results will be saved for viewing. These results can then be translated into visual models and graphs directly in the COMSOL software. These were used to examine the effects of changing variables, such as the bulk feed concentration, to evaluate the model. "Events" are used to define factors that change at a specific time during the model's study such as a spike in

concentration in the bulk fluid after a few hours. This was tested to prove that the model can simulate a change in concentration in the bulk fluid and the effect that will have on the concentration in the hydrogel. Combining these parameters allow for the creation of a transient model that can be used to see long term effects of changes in the environment or hydrogel.

Results

Figure 6 shows a transient diffusion model for ammonia. The concentration at the microbial surface interface and at the bulk interface are graphed over time. This model used the engineering assumption that at time zero ammonia is added to the bulk. After the ammonia is added, the bulk fluid concentration is kept at a constant concentration of 47 mol/m^3 while the ammonia slowly diffuses through the film. Eventually, the model reaches a steady state where the concentration of ammonia at the microbe surface will match the bulk fluid concentration if the bulk concentration is held constant. For this model that point is a little over 1.5 hours calculated from the diffusion coefficient for ammonia through the PEG hydrogel. Hydrogen peroxide without any reaction would eventually reach the same steady state condition where the concentration at the microbe interface is the same as the bulk. The difference in this will be the transient model as hydrogen peroxide has a lower diffusion coefficient and takes around 2 hours to reach steady state. The models average and minimum concentration at the microbe interface reaches the same equilibrium, but this is not true during the transient phase due to the MES shape where the ratio of surface interface to bulk interface is not the same at the corners as the bulk of the MES.

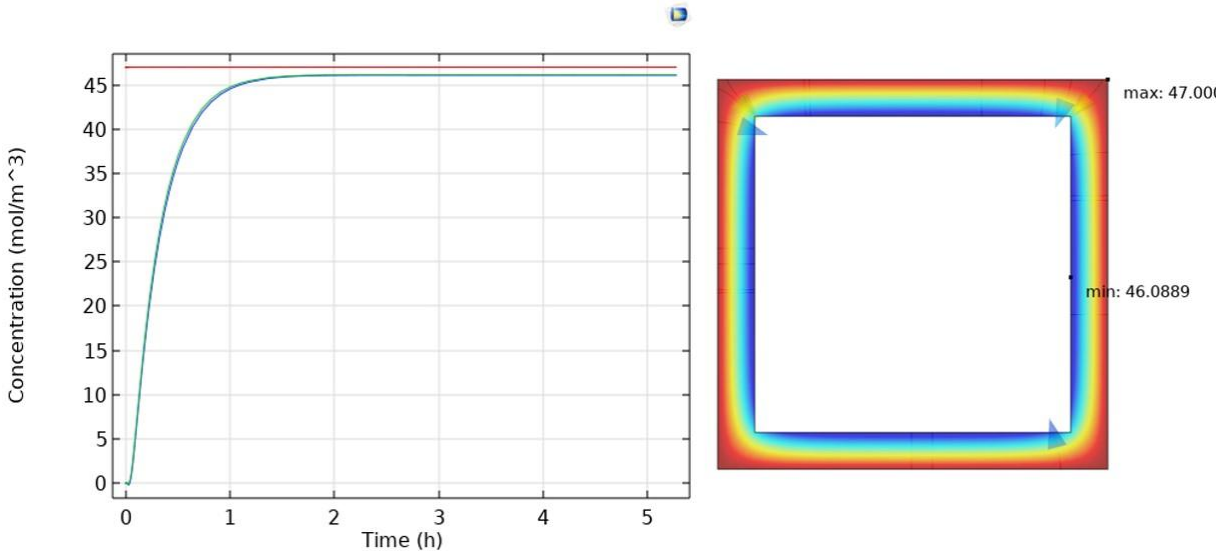
Figure 5 Ammonia concentration over time (red line is concentration at the bulk interface, blue line is minimum concentration at the microbe interface, green line is average concentration at the microbe interface)



Ammonia may be adsorbed and metabolized by microbes at the internal interface. This was modeled by adding a surface reaction rate at the microbe interface. The effect of this can be seen in Figure 7. When the model reaches an equilibrium point between diffusion and reaction the internal interface is a lower concentration than the bulk fluid interface. Additionally, the 2D model on the right shows the concentration gradient after the hydrogel has reached a steady state. This 2D model identifies the cause for differences between the minimum and average concentration at the interface. The dark blue in the concentration profile on the right side of Figure 7 indicates the lowest concentration does not cover the corners completely. This is due to the surface area difference at these corners where the internal surface area is much smaller than the external surface area of the hydrogel. The ratio of bulk increased the diffusion at the corners for this shape. This difference caused by the shape can be important to recognize as the

concentration differences may impact the microbes in the biofilm differentially, depending on the location in the biofilm.

Figure 6 Left) Ammonia concentration over time and right) Ammonia concentration over the hydrogel at steady state (red line is concentration at the bulk interface, blue line is minimum concentration at the microbe interface, green line is average concentration at the microbe interface)

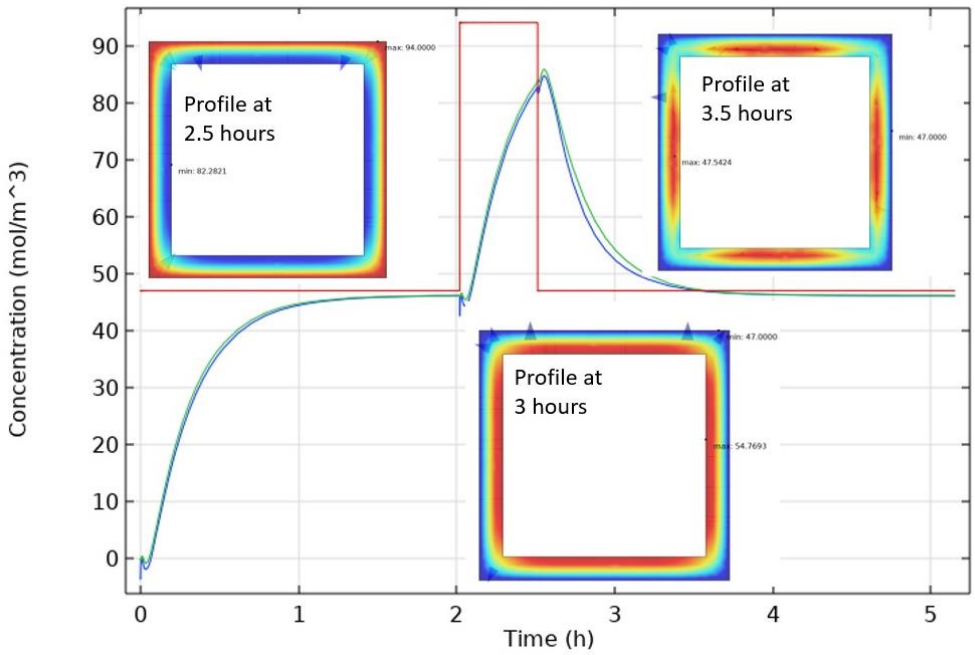


To better simulate the dynamic environment MESs are exposed to, this ammonia model was tested with “Events”. This exemplifies the model’s ability to react to potential environmental fluctuations. Figure 9 shows a system with a spike of ammonia in the bulk fluid for 30 minutes at the two-hour point. This figure additionally shows the concentration profile of the hydrogel during three stages of the reaction to a short spike of ammonia in the bulk. Before the spike occurs, the system reaches the steady state from Figure 8. After the spike, diffusion from the increased ammonia in the bulk gradually increases the concentration at the internal surface. The red line which indicates the concentration in the bulk shows that although there is an immediate increase, the hydrogel slows the increase’s impact on the internal microbes. At two and a half

hours, the spike is no longer in the bulk and the system slowly returns to the previous steady state. In the 2D models little triangles can be identified. These indicate the direction of diffusion. When the bulk is the maximum, the diffusion flows towards the microbes. When the bulk is lower, the diffusion will flow outward. The last 2D images show the transition where the reaction at the microbe interface starts to have a strong impact again. From this, the diffusion will start to shift and return to the steady state.

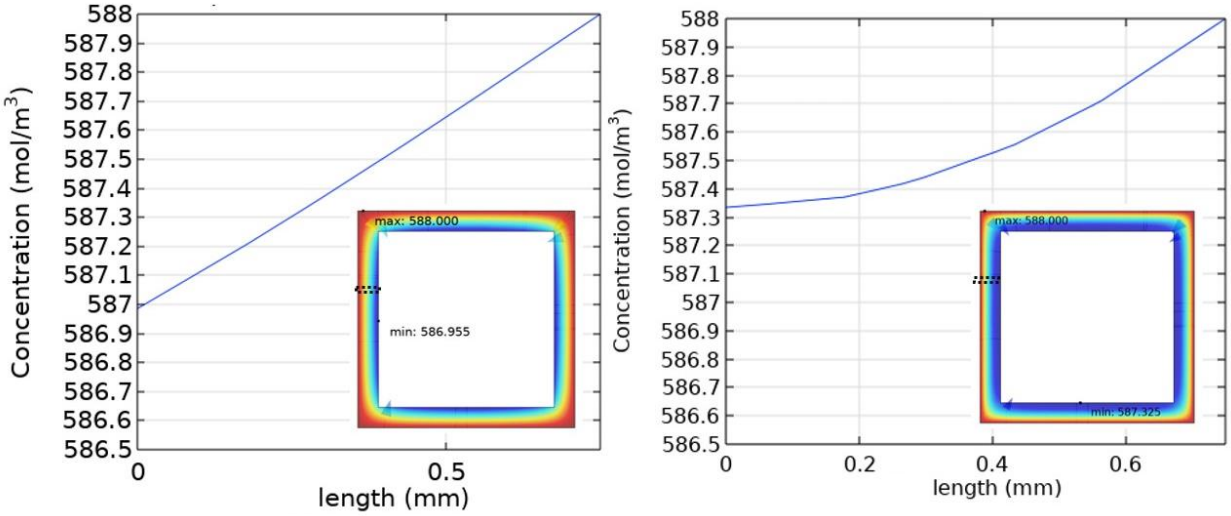
In Figure 8 the difference between the red line of the bulk fluid concentration and the average concentration at the microbe interface shows how the hydrogel is effectively slowing the effect of the ammonia spike. In this simulated event the microbes are never exposed to the full concentration of the ammonia spike as the hydrogel reduces the diffusion so that the time to steady state is longer than the event.

Figure 7 Ammonia concentration over time with a 30-minute spike in bulk fluid concentration two hours into the simulation assuming a MES in a continuous flow environment (red line is concentration at the bulk interface, blue line is minimum concentration at the microbe interface, green line is average concentration at the microbe interface)



The steady state for the two models assuming the same bulk concentration for ammonia and hydrogen peroxide can be seen in Figure 9 below. Although the starting concentration is the same, the profile over the hydrogel at steady state is very different for the two chemicals when reaction occurs. This is because the ammonia has a constant surface reaction rate, but the reaction rate for hydrogen peroxide is in the bulk and dependent on the concentration of peroxide at each location in the hydrogel. In this figure the concentration of the enzyme to react the hydrogen peroxide is very small only $4.4*10^{-5}$ g/mL to demonstrate the difference in profile with a similar overall reaction rate of the stressor affecting the concentration in the hydrogel.

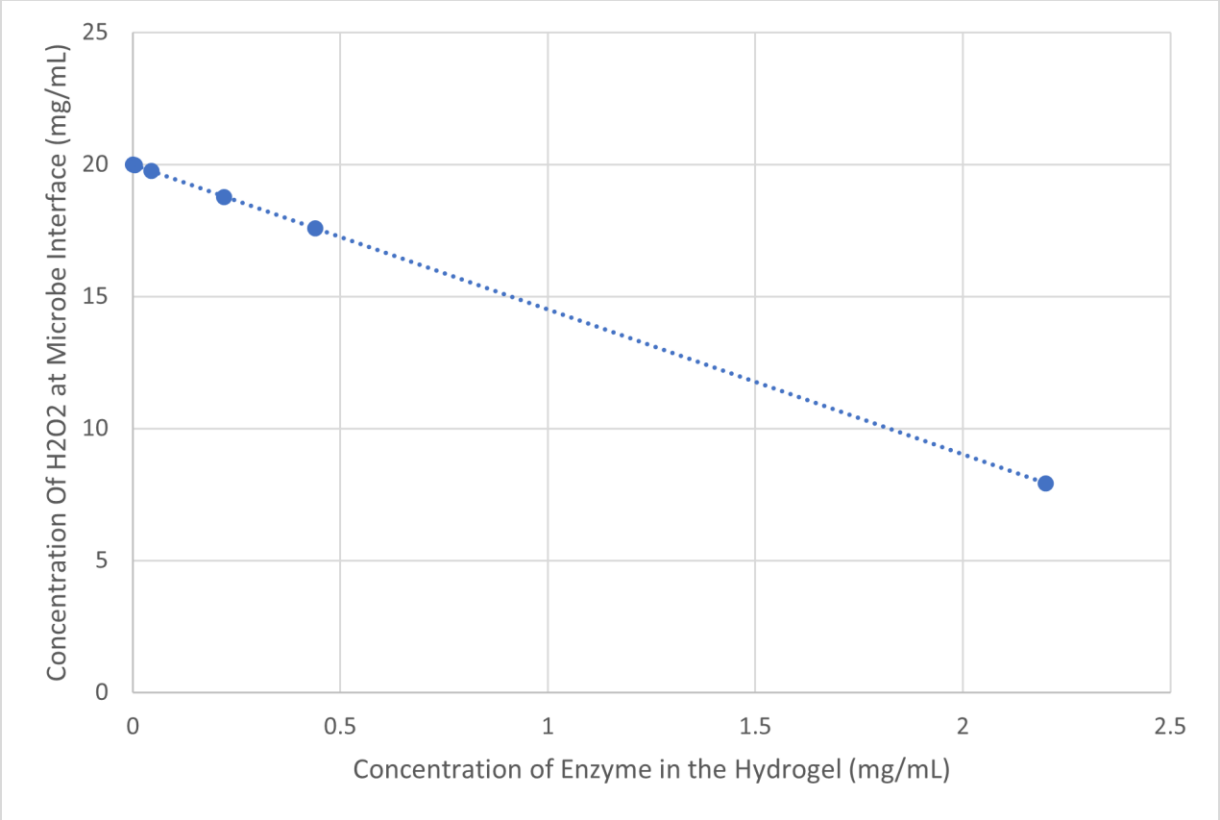
Figure 8 Concentration profile in the hydrogel: left) Ammonia and right) Hydrogen peroxide with an enzyme load of $4.4*10^{-3}$ mg/mL.



Unlike the ammonia surface reaction that is dependent on the microbes the hydrogen peroxide reaction can be increased by increasing the load of the enzyme within the hydrogel. This means that while the hydrogel for ammonia is only effective for handling a dynamic and not steady environment the enzyme loaded hydrogel can be adjusted to be impactful in both steady

and dynamic environments. Figure 10 shows the steady state relationship between the concentration at the microbe interface and the concentration of enzyme in the hydrogel. As enzyme concentration is increased in the simulation, the hydrogen peroxide concentration decreases significantly. This is expected for these values of enzyme because the reaction rate is enzyme limited at these simulation concentrations.

Figure 9 Steady state concentration at microbe interface as a function of enzyme concentration in the hydrogel



Discussion

These results demonstrate the flexibility of modeling a coating for MESs within transient environments. Steady state is achieved after a transient period as shown in Figures 6 and 7 and can be compared to experimental data. This steady state is the maximum concentration the microbial interface will see for the defined system. This model also provides the transient data over time for hydrogel. Using this, the dynamic environment can be simulated by adjusting for factors such as bulk fluid concentration with a simulated temporary spike of ammonia in a continuous flow system as shown in Figure 8. When the bulk concentration increases, the model shows the hydrogel's reaction over time as diffusion increases the concentration in the gel to approach the steady state solution for the new bulk feed concentration. After this spike ends, the diffusion changes direction showing the expected reaction to a drop in the bulk concentration. If the spike was instead a permanent increase in the bulk such as in a batch system, the system would have eventually reached a new steady state solution with a higher concentration at the microbe interface. This proves that the model can be used to provide a more accurate representation of a dynamic environment.

Complex reactions are able to be defined for COMSOL simulations such as Michaelis-Menten in this model. The hydrogen peroxide catalytic reaction with the enzyme has two steps, one of which is an equilibrium step. The reaction dependence can be seen in Figure 9 where the concentrations drop rate tapers as it approaches the membrane due to the reaction slowing from the decreased concentration. The hydrogen peroxide model provides an example of how this simulation software can be used to test various loads of enzymes in a hydrogel such as in Figure 10. This would reduce the material and timeline to optimize a system for various concentrations

of materials. A trend can be defined in simulation and then the optimized system can be tested to confirm the results.

While these two models only include one diffusing component, it is possible to include more to better represent the environment a full-scale system would be exposed to. For example, hydrogen peroxide breaks down to produce H_2O and O_2. By defining the O_2 concentration in the bulk and the diffusion coefficient, it would be possible to see how the reaction affects the concentration in the gel. For anaerobic bacteria where the oxygen should be close to zero in the bulk this reaction and diffusion could negatively impact the bacteria if close to the surface. This type of interaction can be easily paired with events that cause spikes in one component and thereby may cause a chain reaction affect in the gel.

In addition to the flexibility of the modeling software, this software allows for easy visual representation. The data can be used to directly compare concentrations at various points in the hydrogel and keep identical locations run to run. These provide an easy and accurate way to compare specific points for each simulation that will not be affected by potential human or other interactions.

Conclusion

Due to the difficulty in testing large numbers of dynamic conditions in a laboratory setting, the feasibility of modeling these systems using software provides a significant avenue for growth in the field. In this report, it was proved that a model can be generated for a given hydrogel system. This model can be adjusted to account for many environmental and system factors. It was proven that the bulk concentration can be tested for transient and steady state. These models are able to simulate events, such as a spike in ammonia or potential drop in nutrients. COMSOL can be used to model how different components in the bulk fluid will interact with the hydrogel with minimal change to the base model. It is feasible to model a hydrogel loaded with a desired concentration of enzyme to react to a diffusing chemical. With this flexibility, the model has significant potential for future research and can be used to identify what materials are effective in dynamic and steady environments. In this paper this was proved where they hydrogel interaction with ammonia in the bulk fluid showed effectiveness only in the dynamic environment but the loading of the enzyme in the hydrogel to remove hydrogen peroxide showed effectiveness in both dynamic and steady environments. Future research could include a more complex model that records diffusion of more than one component in the system. This could then be used to optimize the PEG coating to give a good design basis to continue more in-depth experiments in a laboratory. Overall, COMSOL software provides a good solution to better understand the effects of a coating for a MES in a dynamic environment.

References

(1) Hernandez, C. A.; Osma, J. F. Microbial Electrochemical Systems: Deriving Future Trends From Historical Perspectives and Characterization Strategies. *Frontiers in Environmental Science* **2020**, *8*, Systematic Review. DOI: 10.3389/fenvs.2020.00044.

(2) Torres, C. I.; Marcus, A. K.; Lee, H.-S.; Parameswaran, P.; Krajmalnik-Brown, R.; Rittmann, B. E. kinetic perspective on extracellular electron transfer by anode-respiring bacteria. *FEMS microbiology reviews* **2010**, *34* (1), 3-17. DOI: 10.1111/j.1574-6976.2009.00191.x.

(3) Schoepp-Cothenet, B.; van Lis, R.; Atteia, A.; Baymann, F.; Capowiez, L.; Ducluzeau, A.-L.; Duval, S.; ten Brink, F.; Russell, M. J.; Nitschke, W. On the universal core of bioenergetics. *Biochimica et Biophysica Acta (BBA) - Bioenergetics* **2013**, *1827* (2), 79-93. DOI: https://doi.org/10.1016/j.bbabio.2012.09.005.

(4) Koch, C.; Harnisch, F. What Is the Essence of Microbial Electroactivity? *Front Microbiol* **2016**, *7*, 1890. DOI: 10.3389/fmicb.2016.01890 From NLM.

(5) Na, S.; Hai, R.; Wang, X.; Li, N.; Chen, D. Concentrations and Seasonal Variations of Perfluorinated Compounds in Sludge from Three Wastewater Treatment Plants in China. *Analytical letters* **2020**, *53* (15), 2400-2412. DOI: 10.1080/00032719.2020.1744161.

(6) Protecting Water Quality from Agricultural Runoff. United States Environmental Protection Agency: EPA.gov, 2005.

(7) Lundberg, P.; Bruin, A.; Klijnstra, J. W.; Nyström, A. M.; Johansson, M.; Malkoch, M.; Hult, A. Poly(ethylene glycol)-based thiol-ene hydrogel coatings-curing chemistry, aqueous stability, and potential marine antifouling applications. *ACS Appl Mater Interfaces* **2010**, *2* (3), 903-912. DOI: 10.1021/am900875g From NLM.

(8) Wang, L.; Li, X.; Sun, T.; Tsou, Y. H.; Chen, H.; Xu, X. Dual-Functional Dextran-PEG Hydrogel as an Antimicrobial Biomedical Material. *Macromol Biosci* **2018**, *18* (2). DOI: 10.1002/mabi.201700325 From NLM.

(9) Parkhey, P. Chapter 11 - Scale-up of bioelectrochemical systems: Stacking strategies and the road ahead. In *Scaling Up of Microbial Electrochemical Systems*, Jadhav, D. A., Pandit, S., Gajalakshmi, S., Shah, M. P. Eds.; Elsevier, 2022; pp 173-193.

(10) Fattahi, N. Hydrogel interfaces for applications in microbial biotechnology. Kansas State University, Doctor of Philosophy, 2021.

(11) Chance, B. THE KINETICS OF THE ENZYME-SUBSTRATE COMPOUND OF PEROXIDASE. *Journal of Biological Chemistry* **1943**, *151* (2), 553-577. DOI: https://doi.org/10.1016/S0021-9258(18)44929-0.

(12) Parameswaran, P.; Zhang, H.; Torres, C. I.; Rittmann, B. E.; Krajmalnik-Brown, R. Microbial community structure in a biofilm anode fed with a fermentable substrate: The significance of hydrogen scavengers. *Biotechnology and bioengineering* **2010**, *105* (1), 69-78. DOI: 10.1002/bit.22508.

(13) G*ases Solved in Water - Diffusion Coefficients*. Engineering ToolBox: 2008.

(14) Coefficient of H2O2 Diffusion. USP technologies: 2022.

Appendix A - Calculations for ammonia model

0.08 g to 0.15g biomass/g acetate consumed[12]

Biomass $C_5H_7O_2N$ MW 113.1146 g/mol

Acetate $C_2H_3O_2$ MW 59.04 g/mol

6.4*10^-6 mol/m^2s acetate consumption – rate from baseline model

Ammonia NH_3 MW 17.03 g/mol

$$\frac{1\ mol\ NH_3}{1\ mol\ C_5H_7O_2N} * \frac{0.08 g C_5H_7O_2N}{1\ g\ C_2H_3O_2} * \frac{1 mol C_5H_7O_2N}{113\ g C_5H_7O_2N} * \frac{59\ g C_2H_3O_2}{1\ mol\ C_2H_3O_2} * \frac{6.4 * 10^{-6} mol\ C_2H_3O_2}{m^2 s}$$

$\frac{2.67*10^{-7}\ mol\ NH_3}{m^2 s}$ $consumption\ at\ surfaces$ worst case

$\frac{5 * 10^{-7}\ mol\ NH_3}{m^2 s}$ $consumption\ at\ surface\ best\ case$

Appendix B - Calculations for hydrogen peroxide model

Standard diffusion rate of ammonia in water $1.5*10^{-5}$ cm^2/s[13]
Standard diffusion rate of hydrogen peroxide in water $1.13*10^{-5}$ cm^2/s [14]

$$\frac{H2O2_{H20diffusionrate}}{NH3_{H2Odiffusionrate}} = \frac{H202_{PEGdiffusionrate}}{NH3_{PEGdiffusionrate}}$$

$$\frac{1.5 * 10^{-5}}{1.13 * 105^{-5}} = \frac{H202_{PEGdiffusionrate}}{NH3_{PEGdiffusionrate}}$$

$$1.32 * 10^{-6} to\ 1.68 * 10^{-6} \frac{cm^2}{s}$$

Appendix C - COMSOL model additional figures

Appendix C Figure C.1 Additional COMSOL examples