ME 450 Final Report
Structural Design and Analysis of Plastic Component Reactors for Solar Hydrogen Production
Winter Semester 2021

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EXECUTIVE SUMMARY

The use of alternative energy sources has been a topic of interest, research, and development for engineers and scientists for many years. Although hydrogen gas is a viable alternative energy source, developing a cost-effective technology necessary for successfully generating H_2 from water remains a difficult challenge. Proposed reactor designs that facilitate generation, storage, and transport of solar energy in the form of stable, energy-dense chemical bonds are gaining traction as a burgeoning technology. However, there remains a lack of knowledge regarding the feasibility of using proposed methods, such as the concept of implementing large photocatalytic flexible plastic reactors for hydrogen production, collection, and transport.

The basis of this project as a whole seeks to address these challenges using sunlight as an alternative energy source, in conjunction with additional soluble redox shuttles, which allow for separate generation of hydrogen and oxygen to mitigate explosive hazards. Existing scientific findings by our sponsors and other interested parties support our ability to propose a prototype device that will use plastic reactors with the mechanisms described to produce the desired hydrogen gas. Furthermore, it is desirable to utilize plastic as the reactor housing in order to maintain a cost-effective approach while generating large amounts of hydrogen from sunlight. The project sponsor has indicated interest in a vertically stacked, two-compartment reactor with a flexible, bag-like design that operates using semiconductor particles and soluble redox shuttles (e.g., salts) to affect the desired chemical reactions to produce the hydrogen. This design potentially offers a tandem and efficient light absorption by the semiconductors, minimizing the square footage of the reactor. However, the full efficacy of the stacked design has practical design aspects that may be difficult to overcome, in addition to a lack of knowledge of using flexible, stacked, transparent plastic bags as reactors to produce, transport and collect hydrogen.

The purpose of this capstone project is to develop a prototype plastic reactor design based on the compilation of various functional needs of this system. Our goal is to perform structural and fluid flow analyses of the materials and reactor infrastructure to identify a practically viable design for a prototype bag reactor that is scalable. Thus, the project entails simulating plastic bag reactor designs with materials, auxiliary components, and support structures as proposed, while providing high-quality documentation. The purpose of this report is to document our analyses and provide our results, findings, conclusions, and solutions. The final design chosen is a semi-rigid plastic reactor with two tandem plastic reactors connected by a porous, semi permeable membrane. The reactor is sized for 1L of fluid with semiconductor particles and redox shuttles dissolved in a water solution. COMSOL simulations confirmed the reactor provides sufficient redox transport to facilitate steady state reactions to produce hydrogen gas, with a float valve collection system that safely collects and vents the product gas with limited gas mixing. FEA analysis confirmed that PET plastic would be a structurally stable material for the frame and allow light transmission. This design was the most effective at achieving all specifications.

PROBLEM DESCRIPTION/BACKGROUND

To design a prototype plastic reactor to isolate usable hydrogen (H_2) from water using redox shuttles. The reactor will be passively powered by sunlight as a clean energy source. The reactor design should maximize efficiency of the desired chemical reactions and, if possible, should be scalable to multiple sized bags.

The project utilizes sunlight to fuel the plastic bag reactors, which contain water, semiconductor particles, and redox shuttles in different compartments. Redox shuttles (D^+/D) and semiconductor particles will be used to facilitate the reactions. The semiconductor particles function as the photocatalyst for the reactions and the redox shuttles act as charge carriers. There will be a porous separator connecting both compartments, allowing for the transfer of hydrogen ions (protons), H^+(aq), and water-soluble redox shuttles, D^+ and D. The isolation of H_2 from water (H_2O) occurs along a chemical pathway between reactions 1 and 5 [1], shown below:

$$O_2\ Evolution\ Compartment: H_2O\ +\ 2h^+ \rightarrow 2H^+ + \frac{1}{2}O_2\ \&\ 2D^+ + 2e^- \rightarrow 2D \qquad (1)$$

$$Net\ O_2\ Evolution\ Reaction: H_2O + 2hv + 2D^+ \rightarrow 2H^+ + \frac{1}{2}O_2 + 2D \qquad (2)$$

$$H_2\ Evolution\ Compartment: 2D + 2h^+ \rightarrow 2D^+\ \&\ 2H^+ + 2e^- \rightarrow H_2 \qquad (3)$$

$$Net\ H_2\ Evolution\ Reaction: 2H^+ + 2hv + 2D \rightarrow H_2 + 2D^+ \qquad (4)$$

$$Net\ Reaction: H_2O + 4hv \rightarrow H_2 + \frac{1}{2}O_2 \qquad (5)$$

Reaction 1 takes place in the O_2 evolution compartment, where the oxidation of water produces $2H^+$ and $^1/_2\,O_2$, with the charge carrier redox shuttle $2D^+$ reducing to 2D by accepting two electrons. Next the charge carriers and ions, like H^+ and/or salt species, transport predominantly by diffusion and/or convection through the porous membrane into the H_2 evolution compartment. Here, electrons are exchanged again, this time moving from the redox shuttles to the H^+ ions, reducing the ions in reaction 3 to produce H_2. The redox shuttle, D^+, having donated its electrons to the H^+ ions, diffuses back into the O_2 evolution compartment through the porous membrane to accept electrons and reduce to D, restarting the reaction cycle all over again. In the ideal model presented, each product gas is produced in its own compartment. This limits the mixing of O_2 and H_2, reducing flammability and the likelihood of combustion in each chamber. Two types of semiconductor particles, suspended in the water in separate compartments, absorb the sunlight, allowing one semiconductor to initiate the overall oxidation reaction (Rxn 2) and the other semiconductor to initiate the overall reduction reaction (Rxn 4).

Figure 1 below shows a simplified model of the overall chemical reaction, as well as a more detailed, technical view of each reaction and molecular pathways in each bag compartment. Transport of the H^+ ions and redox shuttles takes place across the porous separator, which separates the rest of the reaction and products into their respective bags.

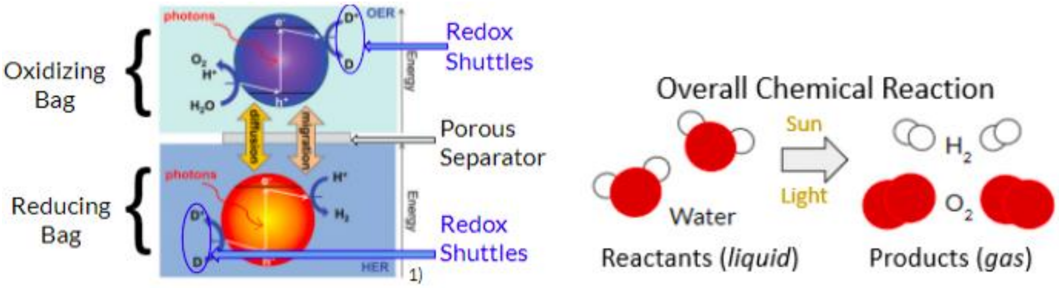


Figure 1. (*left*) a detailed diagram [1] of the compartments which house the reaction oxidation and reduction processes, and (*right*) Illustration of the decomposition reaction of water into H_2 & O_2

REQUIREMENTS/SPECIFICATIONS

Table 1. Requirements and specifications for the structural analysis of reactors

Requirements	Specifications
1. Minimize light absorption and reflection off of plastic, for reactor housing materials.	1. 90% light transmittance in 400-1000 nm wavelength range (visible light)
2. Minimize mixing of hydrogen and oxygen (critical)	2. 4.0% > % of H_2 in O_2 compartment, and 6.0% > % of O_2 in H_2 compartment
3. Minimize energy consumption (critical)	3a. Minimum solar to hydrogen efficiency of 0.1% < Efficiency < 1.0% 3b. If a motor is used, it should not reduce the efficiency by more than 20%
4. Ensure balance of concentration to facilitate transport of redox shuttles (critical)	4. Follow expected daily and steady-state concentrations of shuttles within 10%
5. Multiple scales of the functional system (non-critical)	5. 0.1 L, 1 L and 10 L of water bags

Various functional needs were compiled in order to develop the conceptual design for our plastic bag reactor. The first requirement is to minimize light absorption and reflection from the plastic bag from visible light for the purposes of maximizing light transmission to energize an effective reaction process. This means 90% of light in the visible spectrum (400 to 1000 nm wavelength) must be transmitted through the plastic. The next requirement is to minimize the mixing of hydrogen and oxygen in order to effectively isolate hydrogen for extraction and decrease the chance of flammability within the reactor. The flammability limits based on the volume percent of hydrogen in the presence of oxygen is 4% to 94%. The third requirement is to minimize the consumption of energy in order to have a relatively efficient product. According to our sponsors, efficiency for this product is expected to lie between 0.1% to 1.0%. If a pump is used to facilitate the transport of redox shuttles to fulfill the time limits of diffusion in the second requirement, the efficiency of the entire system must not be reduced by more than 20%. Proper function of the reactor is dependent on a readily available concentration of reactant redox shuttles in each compartment. Originally, our next requirement was to minimize the time required for redox shuttle transport. This was initially set to an arbitrary 5 to 10 minutes to equalize the concentration of the redox shuttles between chambers before redistributing water between the two bags. After further research and discussion with our sponsors, this requirement has been altered. The reactor will still require a balance of concentration of redox shuttles between the compartments, however our new specification to achieve this goal will be to monitor the expected daily and steady-state concentrations. We have developed a benchmark of a range of 10% deviance from steady-state concentration for shuttles in each bag. We will verify that the system meets predicted steady state concentrations through diffusion simulation and calculate the amount of hydrogen produced at a given efficiency for solar energy input to the system. The final requirement is to analyze multiple scales for the plastic bag reactor, and see what changes are necessary for the base design to allow for system scalability. This is consistent with the idea our sponsors have of reactors for 0.1 L, 1.0 L and 10 L of chemical solution.

CONCEPT GENERATION

System Architecture

There are several subsystems involved in the overall system architecture, which can dictate the subsequent requirements and specifications that will be utilized throughout the concept generation process. The first subsystem is the fluid flow subsystem in which the porous membrane facilitates the diffusion of the redox shuttles, thereby affecting the efficiency of the reactor. The needs of the membrane include high porosity and inexpensive, common material. The dimensioning of this subsystem (i.e. the ratio of the separator width to the unit cell width, height of the separator relative to the waterline, etc.) can all be varied in order to maximize the diffusion and flow, while also minimizing the costs of material. The second subsystem is the reactor arrangement itself. The arrangement of the system can affect how much sunlight is able to be absorbed by the redox shuttles, and also affect overall light transmittance throughout the rest of the system. The third subsystem is the structural support, which must withstand tensile stresses in order to maintain a structurally sound system. These three subsystems compose the overall structure.

Fluid Flow Subsystem

Studying the transport requirements and design features of porous membranes to facilitate diffusion between the two reactor compartments led to a few significant discoveries. As Figure 2 shows below, concept generation began from the membrane's requirements and iterated to a variety of material options based on research of current solutions. By referencing what electrolytic materials are successfully used for ion transport in hydrogen fuel cells, (a reverse of the process we are hoping to achieve with our reactors) we found suitable candidates for size-selected transport in potassium hydroxide (KOH), phosphoric acid (H_3PO_4), and specially design proton conducting solid oxide fuel cell separators (PC-SOFC). KOH is the most common electrolytic material used on the market currently, while PC-SOFCs are a newer material that combine high performance with the least degree of heating found in other high efficiency transport membranes. These materials are all suitable candidates recommended to our sponsor. Choosing the correct material for the porous membrane - which will facilitate transport for a specific type of molecule - is critical to maintaining the self-sustaining chemistry in each bag.

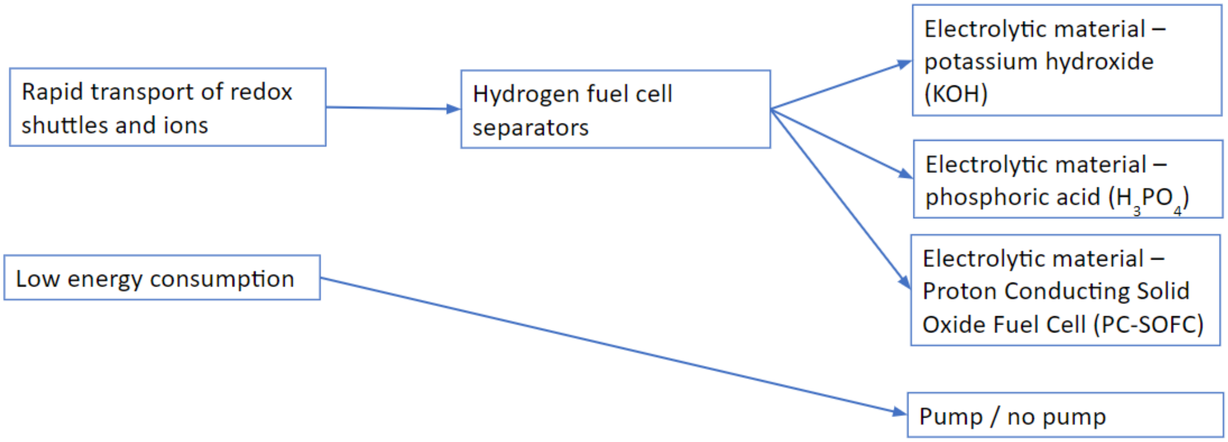


Figure 2. A flow chart of the ideation process for initial porous separator concepts and suitable materials.

Another critical element in the fluid flow subsystem is the need for multiple materials with different connection points for stream flow and ion transfer. Multiple ideas of size-limited and chemical limited transport mechanisms were pitched to the sponsors for feedback. The sponsors informed the team that size-limited transport would be better for the larger redox shuttles because it can isolate select redox shuttles to transport across the membrane. They also informed the team that smaller ionic or proton transport could be achieved both via size and chemical transport. Because of the electrical nature of ion transfer, semiconductor materials could be used to transport electrons or electron holes across a metallic semiconductor without the need for fluid bulk transport of carrier molecules. This led to a dual size-limited and chemical-limited membrane proposed as one option, shown to the left in Figure 3. By the same token, it was also theorized that one single material could be used to transport both species of molecules. This idea of a porous metallic membrane that could chemically transport ions and physically diffuse redox shuttles was incredibly intriguing to the sponsors and is an area of investigation for further development. A version of this combined material design is pictured at the right in Figure 3.

The last element of conceptual design was how to dimension the separators to maximize transport. This primarily came to a few design decisions: 1) the number of transport membranes, 2) the surface area of the membranes connected to each bag, and 3) the length of the membranes between the bags. Having multiple transport membranes is dependent on the need for the design to create the correct stream flow direction. Multiple membranes can facilitate cyclical flow where each membrane has unidirectional flow. A universal membrane would be open to less directional and more bulk diffusion of ions. The other tradeoffs in dimensioning would be the area available for ions to diffuse through. The greater the area, the greater the volume of transport possible. The greater the length, the slower the rate of diffusion transport.

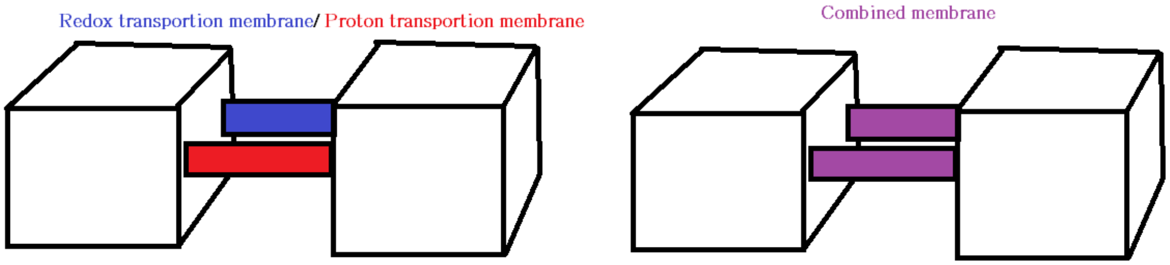


Figure 3. (*left*) A dual, individual ion-specified transport membrane concept for diffusion between the reactors, and (*right*) a combined material membrane concept displaying two membranes for directionality of diffusion and ease of transport.

Compartment Arrangement

The next concept generation process of our design was the bag arrangement and structural support design. Multiple needs were identified through our requirements and specifications which aided our process. Figure 4 visualizes the needs as well as the concepts we generated as a result of the ideation process. Our needs include light transmittance through our material to ensure complete exposure to sunlight for the redox shuttles. Ideation on light transmittance resulted in clear plastic materials that promote light transport. Our needs also include the promotion of rapid transporting redox shuttles, hydrogen production, hydrogen in oxygen concentration maintenance, and gas collection from the system. Our brainstorming process resulted in stacked or hanging compartments to ensure the permeability of particle transport and easy access to the hydrogen gas produced. Our solutions for the bag arrangement design are vertical or horizontal tandem hanging clear plastic compartments. The benefits of the vertical structures are that it increases the surface area and volume exposed to sunlight. However, the horizontal structure increases the ease of transporting redox shuttles. It also creates an easier access to the produced gases with the help of a float valve, which will be discussed in the solution development process. The vertical and horizontal compartments will be further discussed in our concept development process.

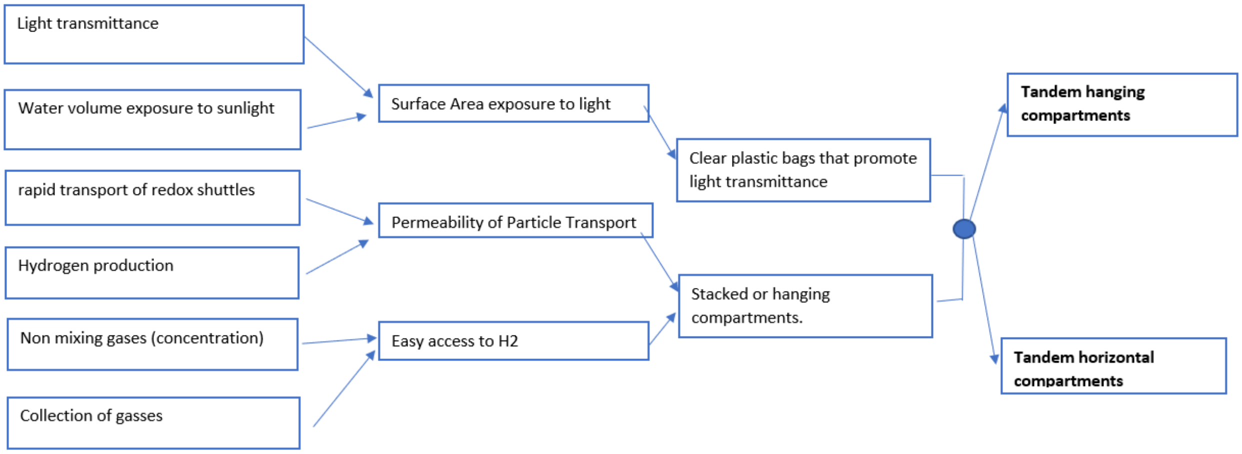


Figure 4. An overview of the ideation process for conceptual solutions for compartment arrangement.

Structural Support

The structural support design has two concept generation processes. The initial process compliments the concept generation for the bag arrangements in the previous paragraphs. The second process was provoked by our sponsors for a flat structure. As seen in Figure 5 below, our initial set of needs for the structural support design includes lightweight materials that can support the tensile stress and weight of the plastic compartments. This was further ideated to the bags being hung by a membrane and structure. Our first possible solution for the 0.1 and 1.0 L compartments is a double plastic bag membrane that resembles a dehumidifier with a plastic hanger. Our possible solution for the 10 L compartments is hollow plastic pipes, which are lightweight and stiffer per unit weight than solid members. Our second set of needs for our structure design is a material that is inexpensive and allows maximal light transmittance. These needs were ideated to compartments that lay flat on the ground. Our solution to this design was a tarp sheet under the bags to prevent punctures. Both solutions will be further examined in our concept selection process.

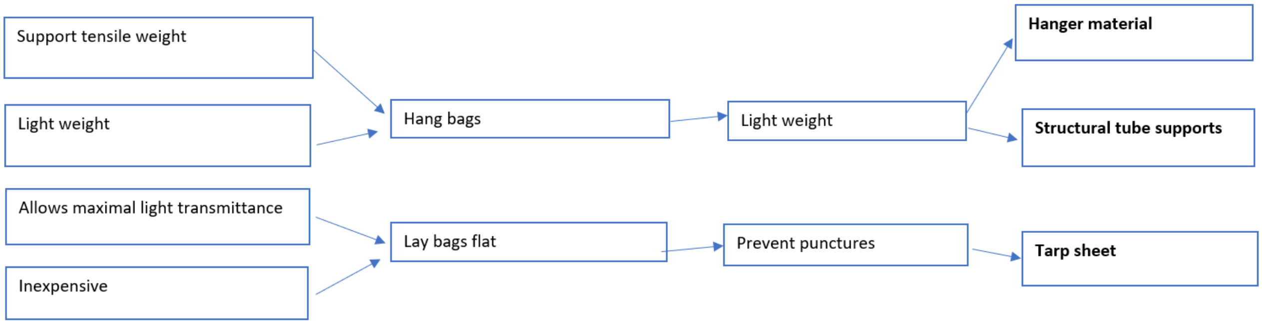


Figure 5. An overview of the ideation process for structural support mechanisms.

CONCEPT DEVELOPMENT

Our initial two design ideas were a tandem horizontally linked structure and vertically linked structure (Figure 6). The advantage of the horizontal design is a lower risk of overmixing of H_2 and O_2. However, there is a disadvantage in its ability to equalize the concentrations between the compartments due to only having a side connection. The vertical bags had a higher risk of mixing H_2 and O_2 due to gas from the bottom compartment possibly moving through the porous separators to the top compartment. However, it has a stronger ability to equalize the concentrations between compartments with its increased area for porous separators.

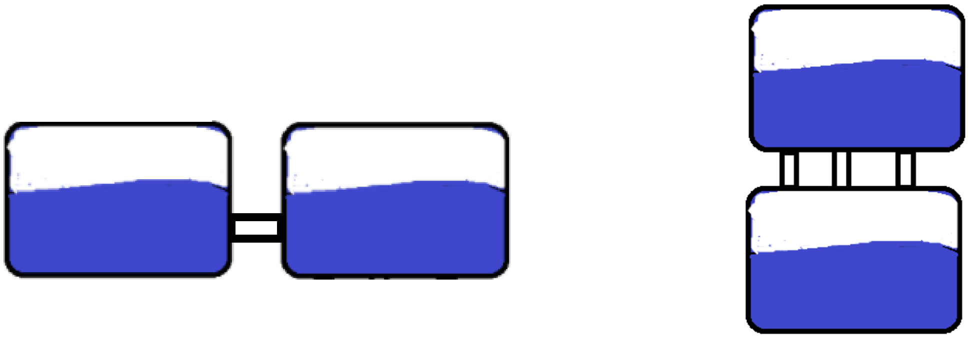


Figure 6. *(left):* Design 1: Tandem Horizontal Hanging Bags. *(right):* Vertical Hanging Bags

Although the functions of our project only structurally required two compartments connected by a porous separator, this allowed us more freedom to brainstorm ideas on the aspects that we still could change. Note that the number of separators is not final. Design 1 (left in Fig. 6) does utilize one whole separator in the figure to maximize diffusion and fluid flow, but Design 2's number of separators is subject to change. This was simply modeled after the sponsors' research, and the team is seeking to verify their design. Since we already had a starting point, we used the design heuristics technique for our concept development, creating new designs by modifying our initial ideas using heuristics given in the Appendix (Figure A.1). Repeated application of different Design Heuristics helped us to visualize how certain features could be changed. Utilizing the Design Heuristics, we brainstormed different ways features can work together and how features could fail in ways we did not anticipate.

To maximize the cost efficiency while still preserving as much sunlight absorption as possible, we took our stacked bag design that would have used external supports and changed it using the "Flatten" and "Remove Material" heuristics, flattening the compartments and removing the external supports (Figure 7). The bags would be laid on the ground with the plastic supporting its own weight as well as the fluid. This would save on any costs that would have been allocated towards manufacturing external structural supports. Sunlight would shine through the top of the bag, which would present the greatest amount of surface area. The porous separators, shown in gray, allow for diffusion between the bags. The gas formed in the bottom compartment would bubble up towards the curved area where it would collect in each pocket. A disadvantage of this design is the increased difficulty in collecting the gases that would form in the bottom compartment, since there is no space above the bottom compartment that would allow for easy access. Another disadvantage is that sunlight would have to penetrate through multiple layers of plastic to reach the bottom compartment, limiting the amount of energy the bottom compartment's photocatalyst can absorb and convert to chemical energy to produce product gas.

Figure 7. Design 2: Flat Stacked Reactor design with gas collection pockets

To minimize the difficulty of collecting gas formed in the bottom compartment, we made an additional change using the "Change Geometry" design heuristic, changing the geometry of the bags to have a triangular shape (Figure 8). With triangular compartments, the gases at the bottom compartment would bubble up towards a corner at the top, allowing for easier access to the gases. This design similarly has the disadvantage of sunlight having to penetrate through multiple layers of plastic to reach the bottom compartment, but has less water to shine through in some areas of the model.

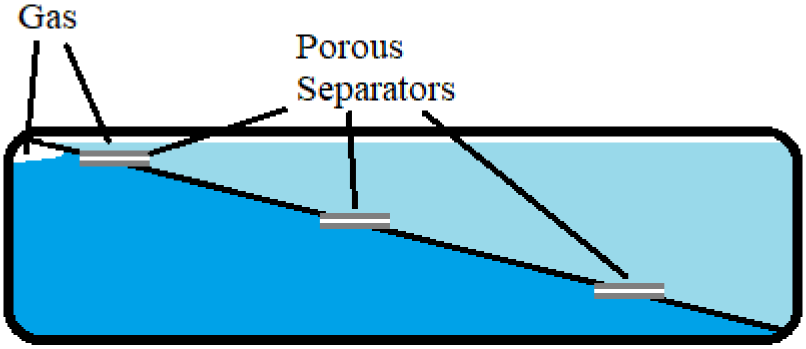
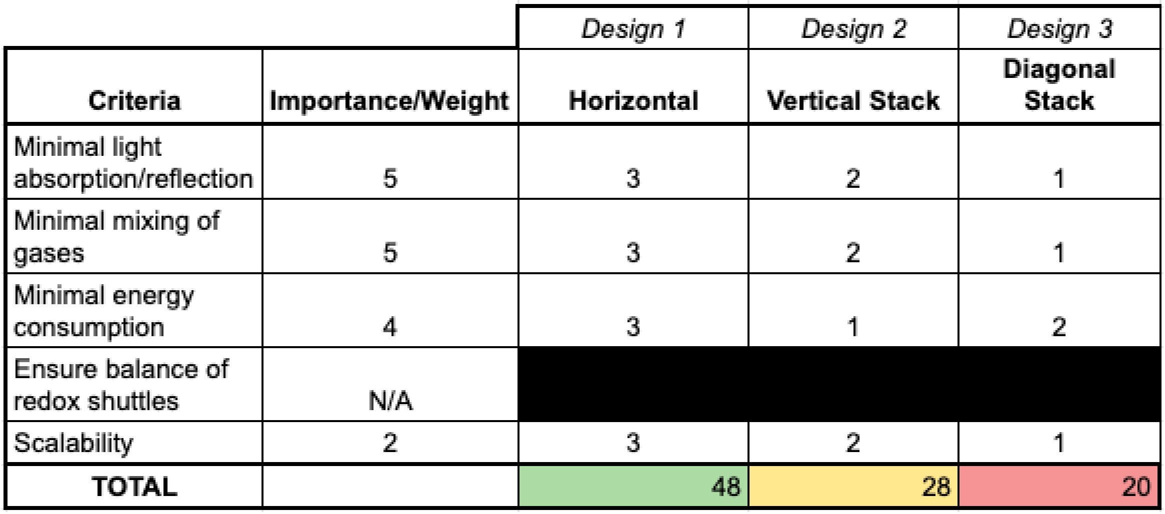


Figure 8. Design 3: Stacked Triangular Bags with corner pocket of gas collection

CONCEPT EVALUATION

The three designs selected for evaluation were: (1) horizontal side-by-side design, (2) vertical long-flat stacked design, and (3) diagonal stack design. These three were selected because of the concept development stage, but also due to the endorsement of Design 2 by the sponsors and the Department of Energy's previous tandem horizontal variation of Design 1. Design 3 was a compromise between the two designs and was developed from applying the design heuristics as previously discussed. In order to evaluate the three designs, the team narrowed down from concept generation and development, a standard metric of comparison was needed. The team decided to use a Pugh chart, and assign weights to different criteria which would affect the overall decision-making process. The top requirements were: (1) minimal light absorption and reflection off of the plastic, (2) minimal mixing of hydrogen and oxygen gases, (3) minimal energy consumption, (4) ensure balance of concentration of redox shuttles, and (5) scalability.



		Design 1	*Design 2*	*Design 3*
Criteria	**Importance/Weight**	**Horizontal**	**Vertical Stack**	**Diagonal Stack**
Minimal light absorption/reflection	5	3	2	1
Minimal mixing of gases	5	3	2	1
Minimal energy consumption	4	3	1	2
Ensure balance of redox shuttles	N/A			
Scalability	2	3	2	1
TOTAL		48	28	20

Figure 9. Pugh chart of the horizontal side-by-side design, vertical long-flat stack design, and diagonal stack design. The horizontal design scored the highest with a 48 overall score.

As evident from the figure above, Design 1 which was the horizontal side-by-side design scored the highest with 48 points. Thus, the team selected it as an initial design to begin the structural design and analysis of the project. However, it is worth noting that the sponsors favor Design 2 because they feel it would minimize the ground surface area the reactor takes up, as well as minimizing the need for structural supports. Redox shuttle balancing was excluded from the design concept evaluation because it is determined the porosity and geometry of the separator, which is a sponsor-specific research development ongoing.

SOLUTION DEVELOPMENT

After the concept selection of the design, the team assessed next steps to ensure a successful transition into the solution development. One such step is to evaluate the initial design using quantitative measurements, which would include force and stress analysis, and calculations of sunlight absorption by the structural materials. In order to conduct force and stress analysis, the team utilized CAD software and finite element analysis (FEA). Furthermore, regarding the sunlight absorption analysis, we seek to use known equations for optical absorption with given absorption coefficients for the structural plastics and water. This would allow the team to determine the percentage of sunlight transmitted through the length of the tandem bag. One item worth noting is that there is no need to analyze how much sunlight would be absorbed by the redox shuttles, as dictated by the sponsors. Our quantitative analysis would provide them with a general sense of the feasibility of the design for their use.

Another step the team has taken is a quantitative and qualitative analysis of the inefficiencies of the system. More specifically, the need for a pump is undesirable, and the team would like to come up with creative alternatives to either limit or eliminate the use of a pump. Creative solutions include the utilization of gravity and tubing to transport the redox shuttles from each reactor. An additional inefficiency or issue with the initial design of the tandem bags is the scalability aspect. In order to solve this problem for each of the three volumes of bags, the team entertained having the same cross-sectional area and varying the depth to accommodate the greater volume of water.

ENGINEERING ANALYSIS

Initial Diffusion Analysis

The simulation tool that the team decided to use for verification of the reactor design geometry for the porous separator was COMSOL Multiphysics. COMSOL is a Multiphysics simulation software that gives users the ability to input or create model geometries, and then test those models with certain physics conditions. COMSOL provides the necessary physics to analyze and ascertain the validity of the teams' reactor design(s). Within COMSOL, a simple 2D model of the reactor system was developed; this 2D model was sufficient because the diffusion analysis was able to test operating conditions on the two primary geometries of the reactor design(s). Geometries were generated for an assumed reactor system of 1 L in size.

The physics selection in COMSOL used was 'Transport of Diluted Species' (TDS). Diffusion is the principal behavior of the reactors; species should flow across the 2D porous membrane and facilitate the chemical reaction generating hydrogen and oxygen. The diffusion physics require concentration-based flow; the diffusion physics are affected by the 2D model geometry, mainly the porous separator. The rate of diffusion across the design separator is the main structural determinant of the efficiency of the reactor's chemical processes.

The COMSOL physics operation relies on a multitude of different model parameters that were specified in the system after the selection of TDS physics. The main parameters of the simulation are the initial concentrations of the D^+/D redox species; in our analysis we assumed these to be Fe^{3+} and Fe^{2+}. Other model parameters necessary to run this simulation include: the volumetric dimensions (reactor length and width scale, with an assumed depth of 5 cm), the porosity of the separator membrane, the concentration generation of redox species, and the consumption rate of the redox species. These parameters were useful in the pursuit of determining the most effective width-ratio, the ratio between the width of the porous separator and the unit cell of a reactor compartment. Data was obtained from the Bala Chandran research paper concerning the theoretical model of the reactor system [1].

In order to verify that the dimensions of our proposed designs can facilitate redox shuttle diffusion suitable for each reactor's operation, we developed a simplistic COMSOL model to measure the diffusion rates and molar changes in redox concentrations. By analyzing the system in 2D, we were able to test different operational conditions for the two primary geometries in our designs, mainly that of a full-length porous membrane and that of three limited, separated membranes for Designs 1 and 2, respectively.

By simulating conditions relevant to the expected size of a 1 L system, we were able to see if our proposed design would match the expected behavior of the theoretical system developed by our sponsors. Because diffusion is principally a concentration-based flow phenomenon, the geometry and availability of flow path for dissolved species, such as redox shuttles, affects the rate of diffusion and ultimately affects the efficiency with which the reactions can be self-sustaining. Self-sustaining reactions are important to the system's operation for the ultimate intention of the system to be a passive system, with little external input from the user. Based on our sponsor's analysis [1], 1 L systems of 5 cm depth of fluid should begin operation at concentrations of 0.7 M (mol) of each redox shuttle throughout the system and should reach a steady state operational concentration of 1.05 M or 0.35 M, depending on if the redox shuttle is in its dominant reactor. This means the D^+ shuttle should reach ~1.05 M in the hydrogen compartment and ~0.35 M in the oxygen compartment. The D shuttle should reach ~1.05 M in the oxygen compartment and ~0.35 M in the hydrogen compartment. Steady state concentrations and self-sustaining reactions should be achieved between 50 and 75 days of passive operation for this scale of reactor. Using Figure 5c of the Bala Chandran paper [1], as well as additional diffusion data and sizing specifications, a COMSOL model was achieved for each of the design geometries proposed from our CAD models.

Given the expected results above, the COMSOL model for Design 1 performed within specifications. Below is a visualization of the concentrations of each redox shuttle over 100 days of operation, with color grading used to show the concentration of each redox species in moles (M). In each visualization, the leftmost compartment is the hydrogen reactor, while the rightmost compartment is the oxygen reactor, with the porous membrane in the middle. The animation on the left represents the concentration of a proposed Fe^{3+} (D^+) ion, and the animation on the right represents the concentration of a proposed Fe^{2+} (D) ion. The animation iterates through 100 days, with each frame representing one hour. Figure 10 shows the COMSOL analysis of Design 1:

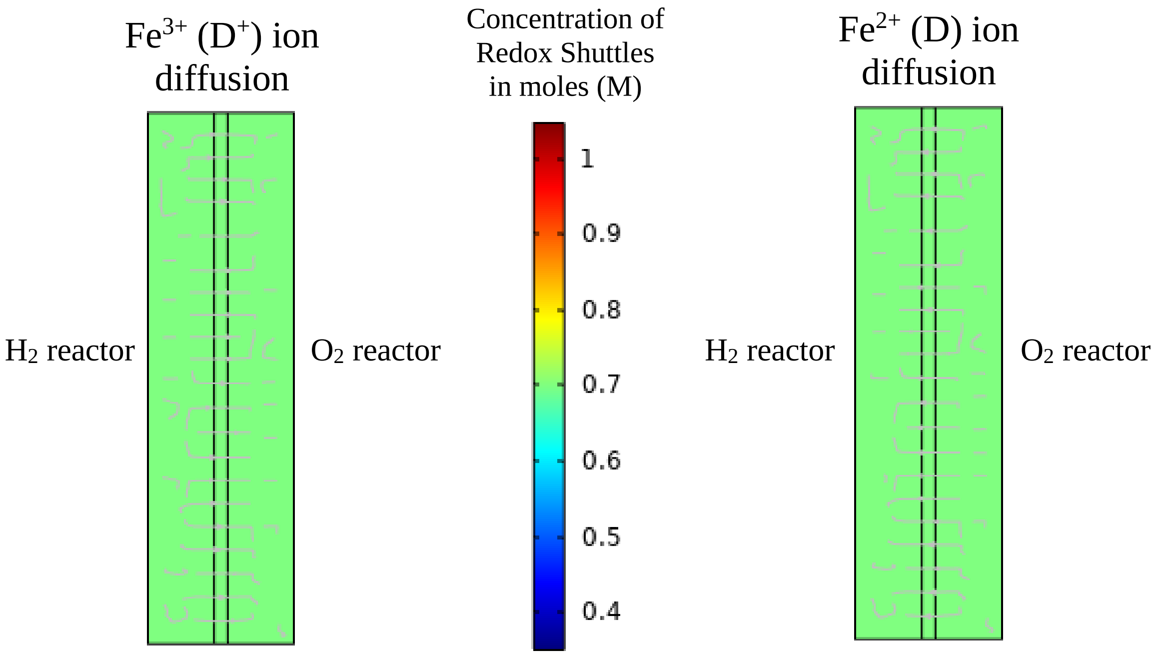


Figure 10. COMSOL model of redox shuttle diffusion in Design 1, showing change in molar concentration over a 100 Day operation. Initial concentration was set to 0.7 M for both redox species, resulting in a net change of 0.35 M for both species in each compartment, within expected operational limits.

Design 1 was a suitable fit for all the expected operational limits for normal operation of the system from initial startup at even concentrations to steady state operation at the separated concentrations of each species in each compartment. Figure 11 below shows the concentration of each species in its dominant compartment (where concentration increases from startup) on the left, and its non-dominant compartment (where concentration decreases from startup) on the right, showing consistent behavior to that of Fig 5c on page 14 of the Bala Chandran paper [1]. Note the concentration is given on a per volume basis, which is a factor of 1/0.0014 larger than the molar concentration scale used in Figure 11.

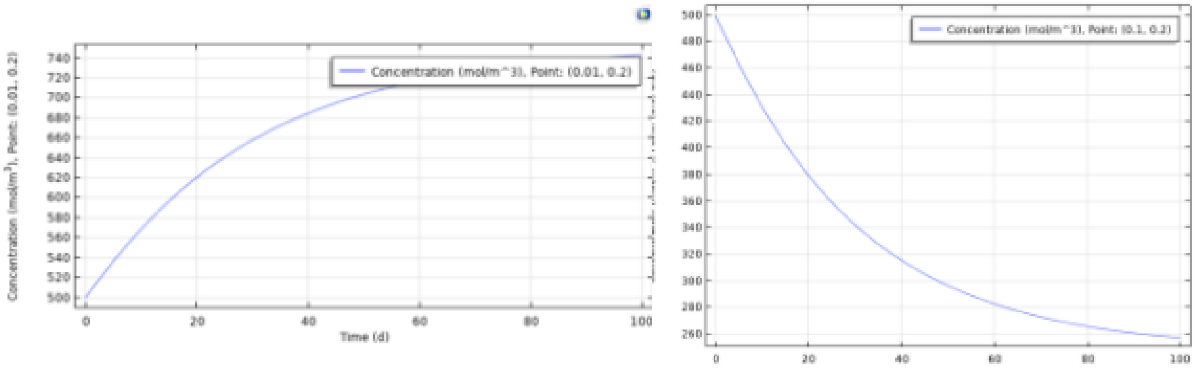


Figure 11. COMSOL plot of redox species concentration vs. time for Design 1, showing the increase in shuttle concentration in the dominant compartment (left) and the decrease in shuttle concentration in the non-dominant compartment (right) for 100 days of system operation

Design 2 differed from Design 1 due to the limited space available for diffusion between reactors as a result of the gas collection pockets of the bottom reactor and had a noticeable effect on the balance of redox shuttle generation and consumption. Whereas Design 1 facilitated even transport across the large membrane, Design 2 had much more limited transport due to the smaller spaces available for diffusion between the reactors. This led to uneven buildup of redox shuttles in their dominant compartments, and a starvation of products in the other reactor compartment due to the limited transport. This is visible in the model by the increased concentration of redox shuttle in its reactant compartment and lack of concentration in its product compartment, meaning the delay in transport can cause the reaction to fail to be self-sustaining. The visualization of the COMSOL sim of Design 2 is shown below, similar to Figure 10 in layout but with different membrane dimensions, and a different molar scale:

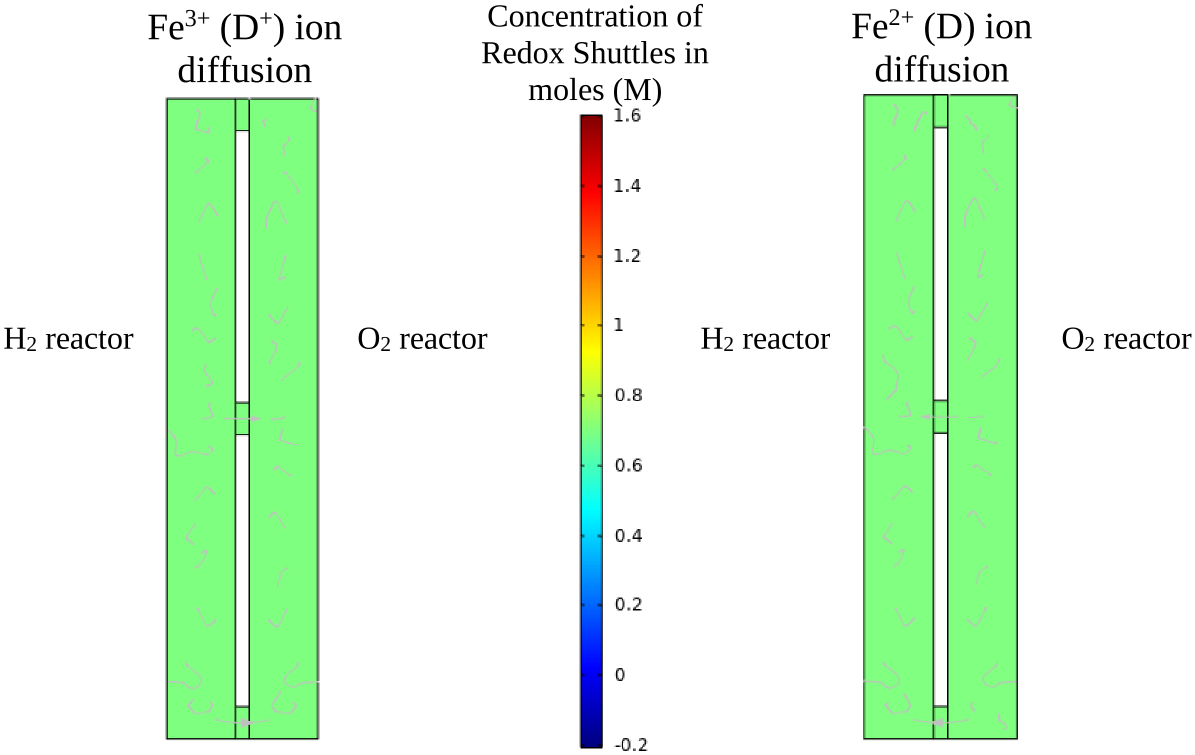


Figure 12. COMSOL model of redox shuttle diffusion in Design 2, showing change in molar concentration over a 100 Day operation. Initial concentration was set to 0.7M for both redox species, resulting in a net change of around 0.9M for both species in each compartment, resulting in a complete consumption of both species around day 90.

If sufficient transport is not achieved, the system will starve itself of reactants in the necessary compartments, and the concentration of each species in the non-dominant reactor will drop below operational limits. Figure 13 below shows the concentration of species in its non-dominant compartment (where concentration decreases from startup), indicating that each species will become used up (concentration will be 0 M or less) by the 90th day of operation, a critical failure of operation. Note the concentration is given on a per volume basis, which is a factor of 1/0.0014 larger than the molar concentration scale used in Figure 13.

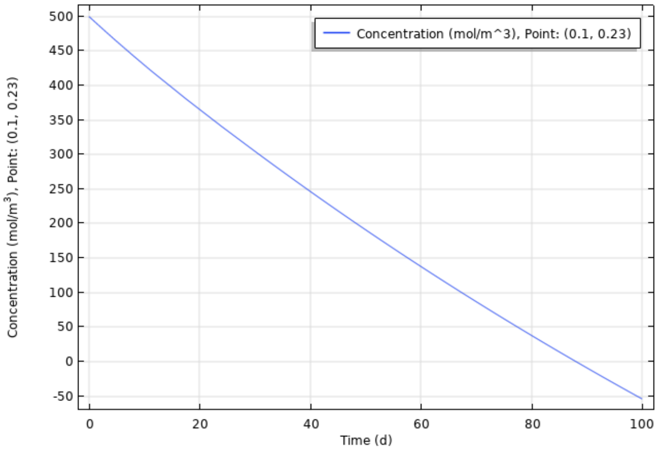


Figure 13. COMSOL plot of redox species concentration vs. time for Design 2, showing the decrease in shuttle concentration in the non-dominant compartment for 100 days of system operation. Notice that the concentration dips below 0M around the 90th day, indicating that the reaction has stalled completely.

Since there is no physical meaning to a negative concentration of dissolved substance, what Figure 13 clearly indicates is that membrane transport of redox shuttles is not at a sufficient rate to allow for a suitable amount of shuttles to act as a reactant and allow the reaction to continue occurring. Therefore, Design 2 is not suitable for operation of the system.

Further study of the ratio of the membrane length to the overall reactor length is given in the Recommendations section on page 29-30. The failure of Design 2 to provide sufficient transport at a length ratio of 1:6.67, and the success of Design 1 at a 1:1 length ratio, clearly indicates that the best possible design is to allow for as great a membrane area as possible, up to a ratio of 1:1.

Initial Structural Design

The team narrowed down the engineering analysis to two designs. The first design is a tank with two side-by-side compartments connected via a porous separator between them (Fig 14). The second design is a stacked tank with porous separators and curved portions for gas headspace between the compartments (Fig 15).

The advantage of the first design is a low risk of overmixing of H_2 and O_2, a large amount of area for porous separators, and low difficulty of manufacturing. However, there is a disadvantage in its ability to equalize the concentrations between the compartments due to only having a side connection.

The disadvantages of the stacked, vertical design are the increased difficulty in collecting the gases that would form in the bottom compartment, that sunlight would have to penetrate through multiple layers of plastic to reach the bottom compartment, higher difficulty of manufacturing, and reduced area for porous separators due to the need to maintain a water level above the porous separators to facilitate diffusion and headspace for gas to bubble up.

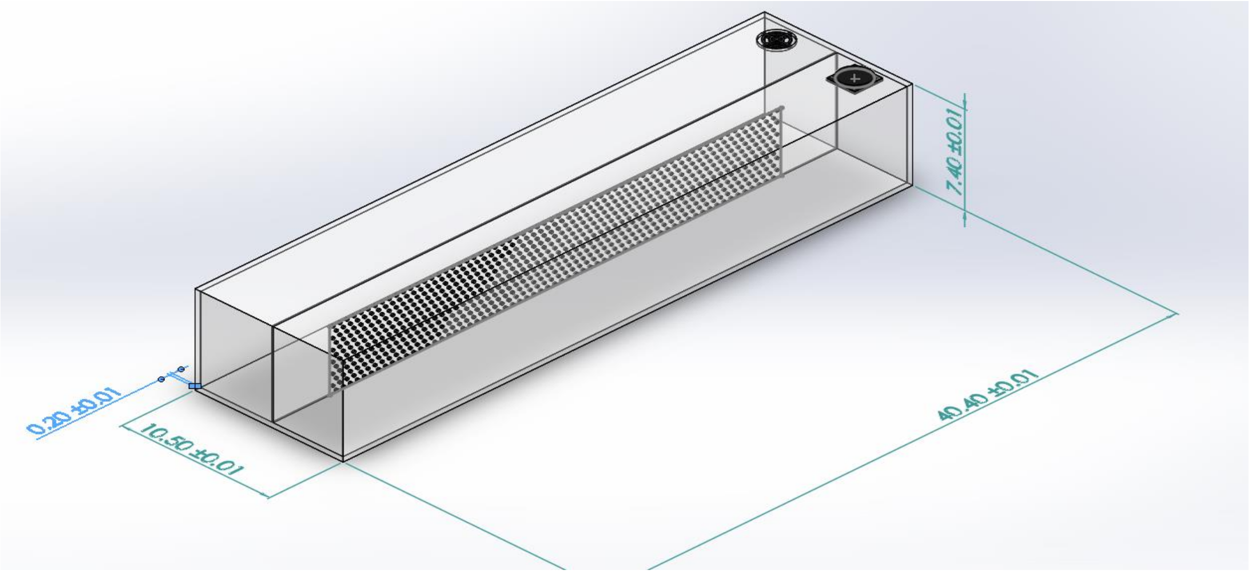


Figure 14. CAD of Design 1 with dimensions with a single 32cm porous membrane

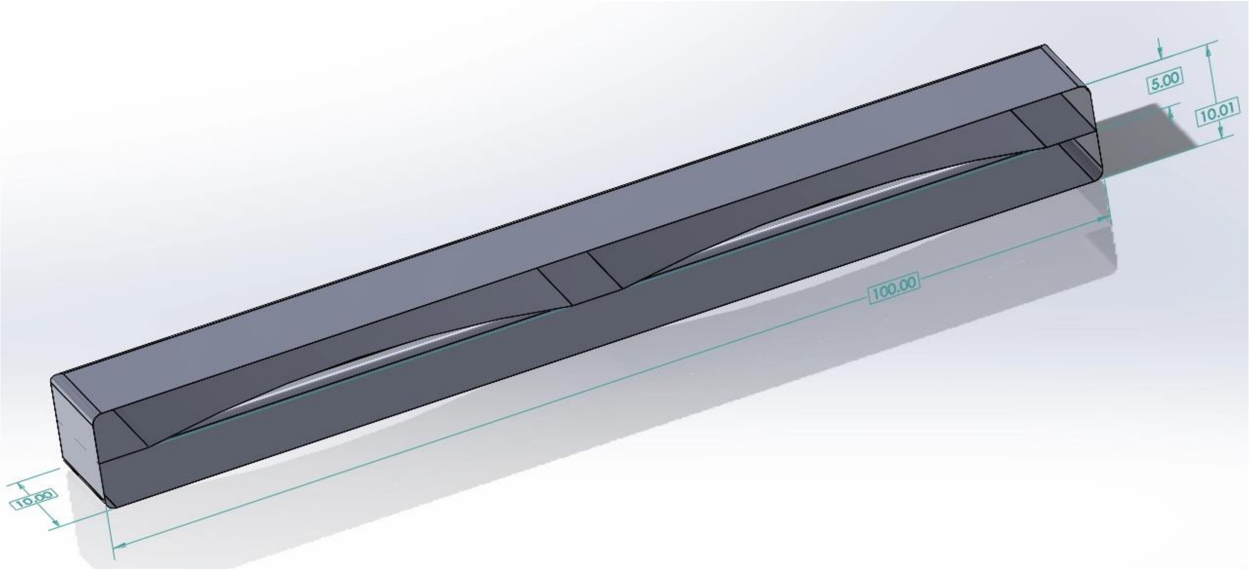


Figure 15. CAD of Design 2 with dimensions, featuring three separated 5cm long porous membranes

Initial Structural Analysis

Structural analysis was done on the designs using Finite Element Analysis (FEA). The loads used for the simulation are gravity forces on the structure and hydrostatic pressure along the inside the tanks. This allows us to simulate the weight of the structure itself along with the weight of the water inside the tanks. There was also a floor constraint on the ground to mimic the ground under the tanks. We chose to test acrylic plastic (PMMA) and high-density polyethylene (HDPE) as both were considered good options structurally and for light transmittance.

The results for acrylic and HDPE lead to similar results for the first design (Fig. 16 & 17). The top of the tanks has been hidden for visibility of the inside of the tanks. The stresses are greatest at the bottom of the outer walls of the design. This is due to the hydrostatic pressures being greater at greater depths, making the bottom of the tanks experience the greatest stresses.

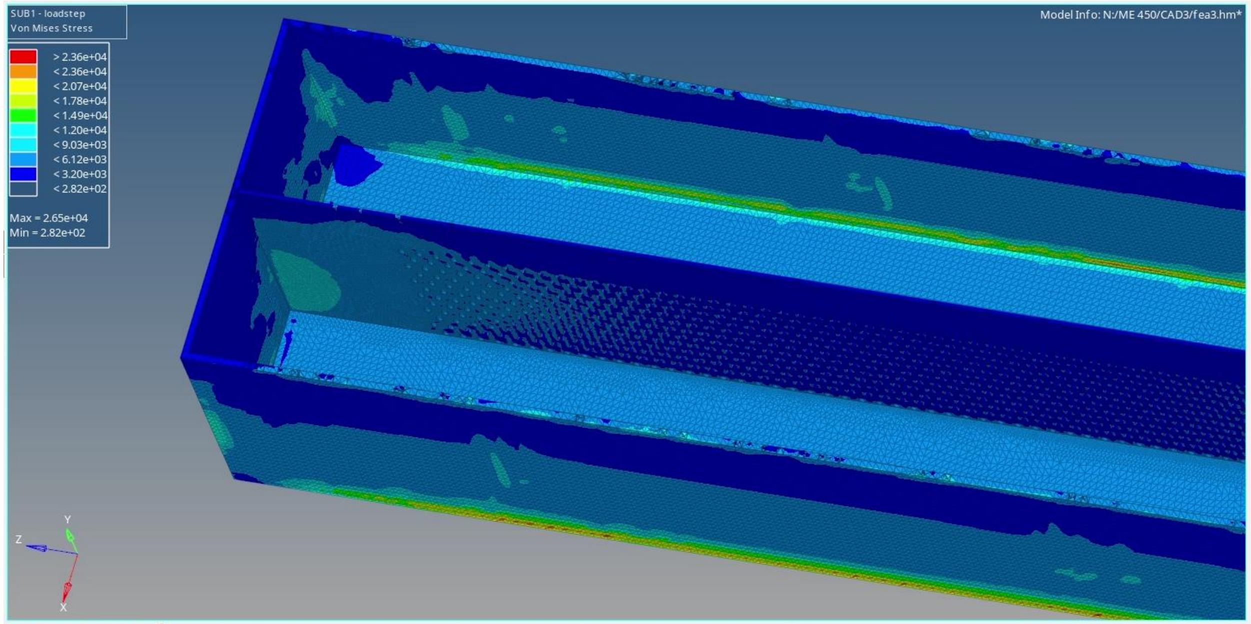


Figure 16. Design 1 HDPE Finite Element Analysis. Max Von Mises Stress found to be 26.5 kPa

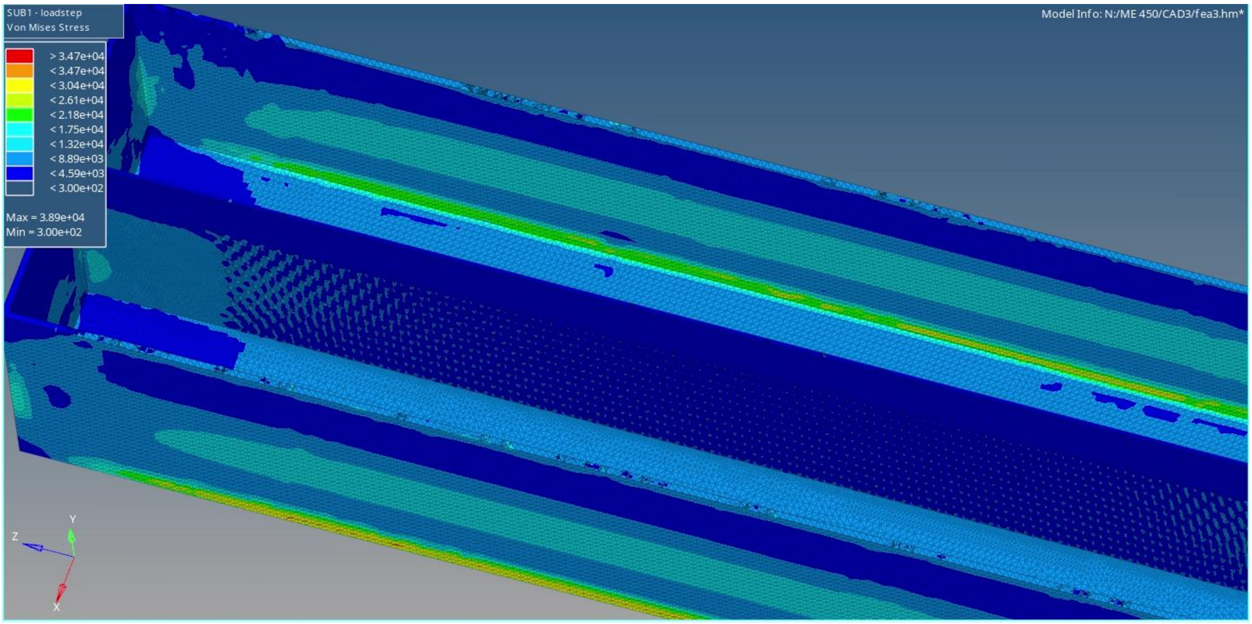


Figure 17. Design 1 Acrylic Finite Element Analysis. Max Von Mises Stress found to be 38.9 kPa

We tested Design 2 using HDPE (Fig 18). The results are similar to the 1st design, where the greatest stresses are located at the bottom portion of the walls of the tanks. The middle support area does not experience much stress due to it being supported through hydrostatic pressure by the water under it.

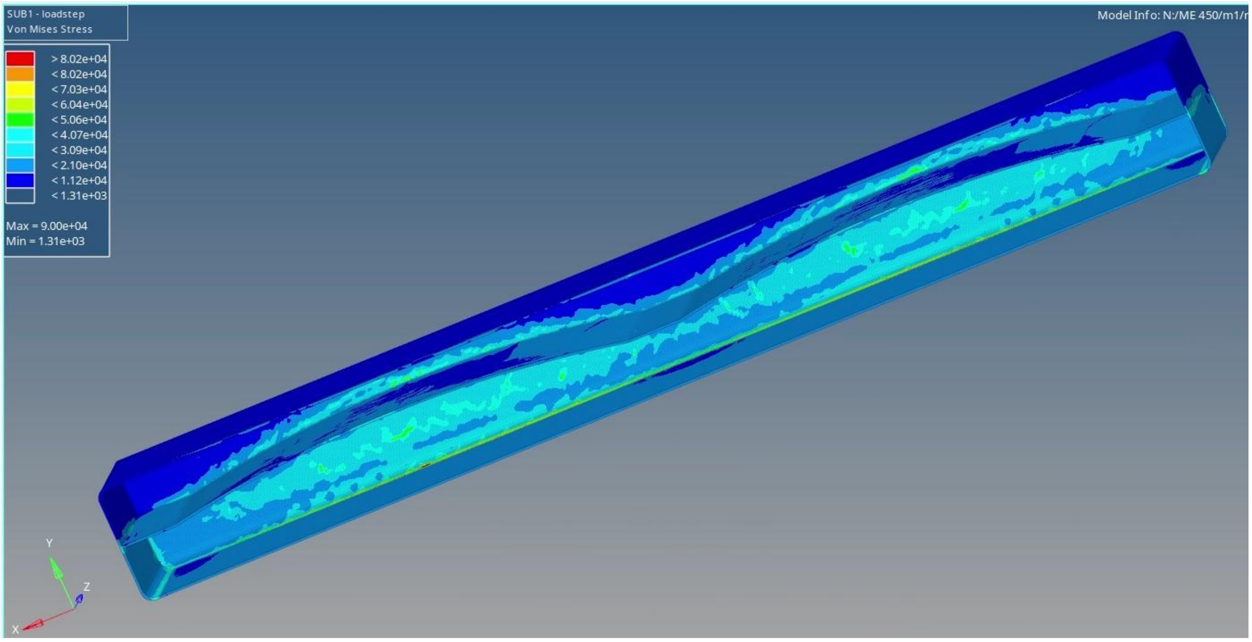


Figure 18. Design 2 HDPE Finite Element Analysis. Max Von Mises Stress found to be 90 kPa

For Design 1, the max Von Mises Stress was found to be 38.9 kPa for acrylic and 26.5 kPa for HDPE. For Design 2, the max Von Mises Stress was found to be 90 kPa for HDPE. The designs currently do not come close to yielding. HDPE yields at ~30 MPa and PMMA plastic yields at ~90 MPa. We can still decrease the thicknesses of the tanks without having stresses large enough for yielding of either material.

Risk Assessment

Based on the FEA, there is no risk in structural failure of the reactor. However, we believe there are some possible risks in the loss of hydrogen gas permeating through the walls of the reactor. This risk is dependent on the gas permeability of the material used for the reactor. Table 3 shows the H_2 permeability coefficient of some plastics. The process of creating hydrogen is slow due to reactants having to travel between two compartments and the hydrogen left in the reactor can permeate through the walls of the reactor. The maximal loss due to permeability is calculated to be 4.95e-9 mol/s for a material selection of LDPE, assuming atmospheric pressure, using the 2 mm thickness and 0.03 m^2 surface area of the H_2 compartment. For materials HDPE, PET, and PMMA, the H_2 loss is calculated to be 1.23e-9 mol/s, 0.183e-9 mol/s, and 1.86e-9 mol/s, respectively. Therefore, it is assumed that H_2 loss is negligible. The upcoming float valve addition is a design change to reduce this risk. In order to minimize the loss of hydrogen, the gas can be collected as it is produced. In our finalized design, the float valve would regularly open to release an accumulated amount of hydrogen produced from the reactor. This feature allows for the hydrogen to be released from the reactor to a separate collection tank or pipeline without any need for direct handling by operators or overseers. Sponsors are free to design additional collection infrastructure as best pertains to their vision of the finalized system, and output of the float valve is adaptable to various threaded or other piping connections, rigid or flexible.

DETAILED DESIGN SOLUTION

Finalized Design

Our finalized design is a 10 cm wide PMMA plastic container that facilitates transport of redox shuttles by minimizing light absorption for reactor housing materials and promoting natural diffusion concentration balance. The oxygen and hydrogen compartments are separated with a one millimeter porous membrane. A float valve was added to the reactor to allow for continual collection of any hydrogen produced. The height of the hydrogen compartment is 5 centimeters while the height of the oxygen compartment is adjusted to the float valve at 9.33 centimeters. The oxygen water line ensures that water fills the float valve to initiate its venting process. The hole on the oxygen compartment is for venting oxygen gas to the atmosphere and can be used for refill purposes. The cap on the hydrogen compartment is for sealing the compartment for gas collection, and can be opened for replenishing water, photocatalysts, and redox shuttles.

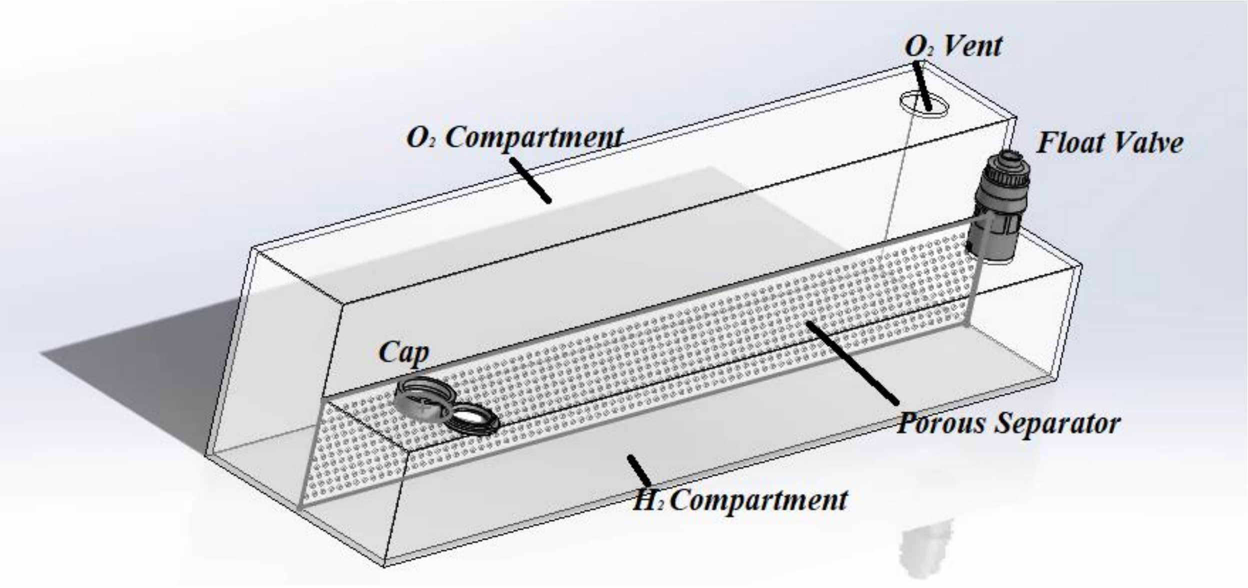


Figure 19. Finalized design of reactor, complete with float valve collection system and filling caps

Flow Valve Design

For the hydrogen collection process, the team chose to install a float valve to our design. In order to initiate the venting sequence, the oxygen water line will need to ensure that water fills the float valve. As hydrogen is produced and displaces the water, the water level lowers. The float ball follows the water level, which when lowered forces the cage downward to open the valve at the top for hydrogen collection. The hydrogen begins venting at a pressure of 96.5 kPa, which is approximately 10.67 mL of gas. The venting pressure was calculated by using Bernoulli's equation to solve for the water pressure in the float valve in relation to the water pressure in the O_2 compartment. Z_1 and Z_2 represents the change in water level, P_1 represents the water pressure at the top of the oxygen compartment while P_2 represents the water pressure predicted at Z_2 after hydrogen is produced. This can be visualized using the Figure 20 below. The volume of hydrogen released was calculated by using the ideal gas law equation. We used standard room temperature along with the pressure at P_2 and the hydrogen moles produced for 10% solar to hydrogen efficiency.

$$P_2 = \frac{m_2 g \left(\frac{P_1}{\frac{m_1 g}{V_1}} - (\Delta z) \right)}{V_2}$$

$$\frac{\left((.02265(\mathrm{kg})) \cdot 9.8\left(\frac{m}{s^2}\right) \cdot \left(\frac{101000\left(\frac{N}{m^2}\right)}{\frac{.8(\mathrm{kg}) \cdot 9.8\left(\frac{m}{s^2}\right)}{.0008\left(m^3\right)}} - 0.022256(m) \right) \right)}{.000022658(m^3)} = 100746.3\ Pa = 14\ \mathrm{Psi} = 96.5\ \mathrm{Kpa}$$

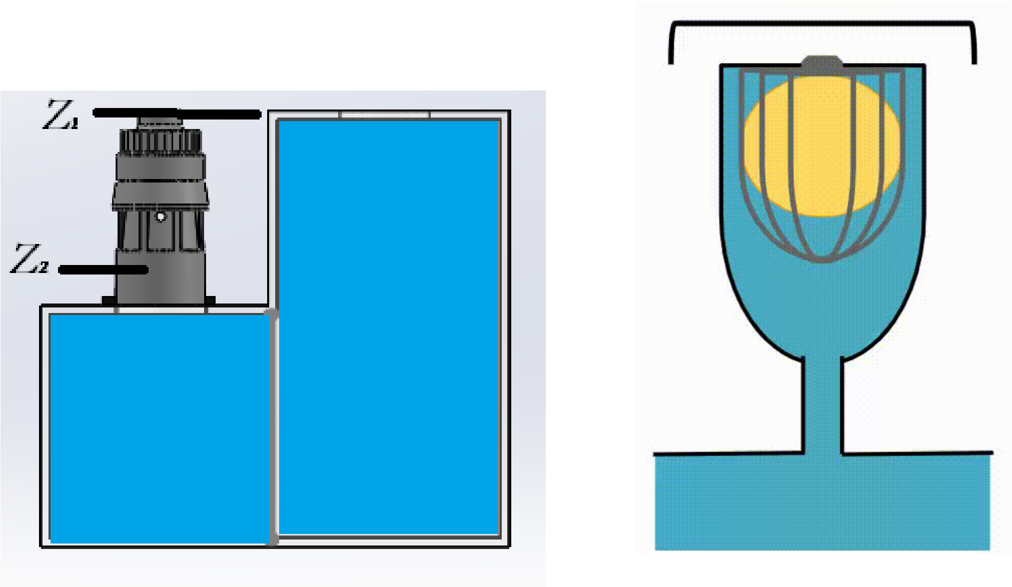


Figure 20. (*left*) Schematic of reactor with water levels used in above calculations labelled, and (*right*) Animation of the filling and emptying float valve, starting at empty, filling with hydrogen forcing the float down, lowering the cage and opening the valve, venting the collected gas.

VERIFICATION

Validation of Finalized Design with COMSOL

To verify that sufficient transport of redox shuttles could occur with our final design, the testbed COMSOL model used previously to test the performance of Design #1 and #2 in DR3 was modified to take on our final geometry. Using the same base parameters - including 0.7M (or 700M/m^3) initial concentration for both shuttle species in each compartment, 8.43e-5 M/m^{3}s volumetric rate of reaction for both species in both compartments (for 1% solar-to-hydrogen efficiency), and base effective diffusivity coefficient of 1.68e-10 m^2/s for the membrane material - the following results were obtained for a side profile cross-sectional view of the finalized design geometry.

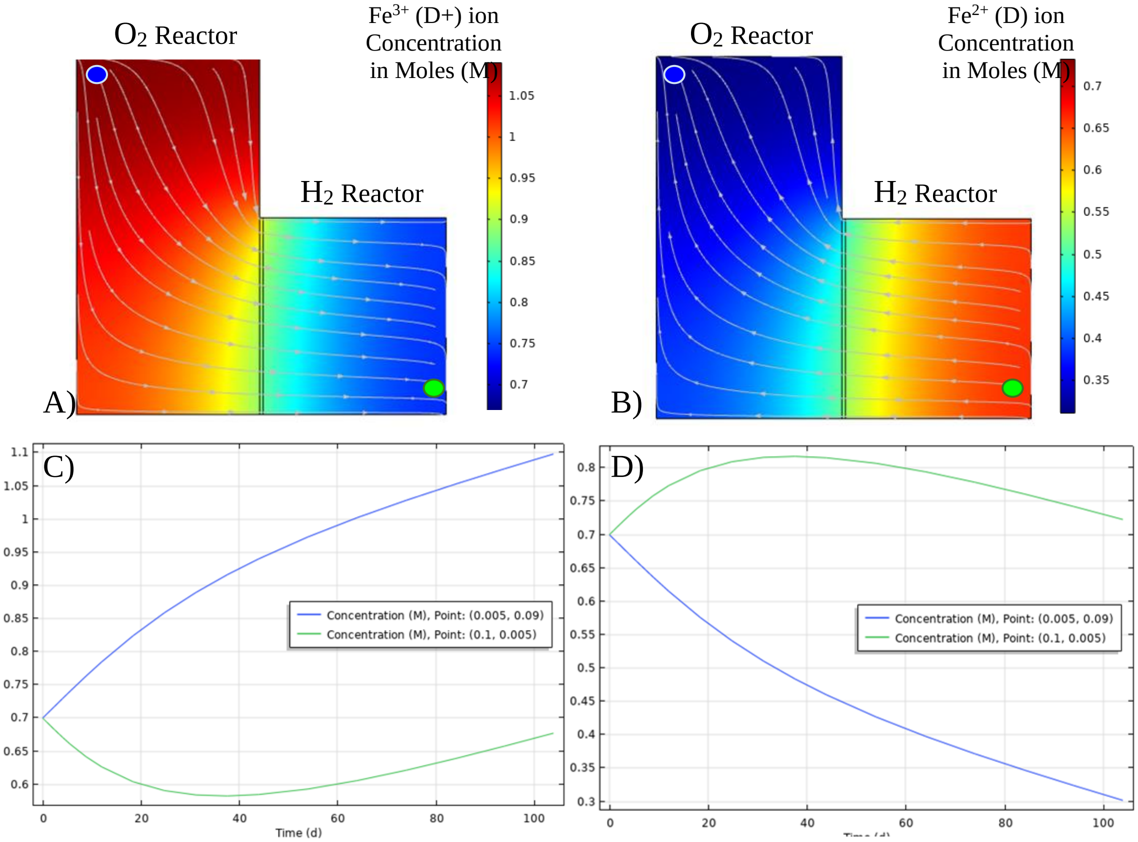


Figure 21. COMSOL Analysis graphics and plots of redox shuttle concentrations over space and time
A) Concentration colorized gradient of Fe^{3+} (D+) diffusion for finalized design geometry at T = 100 days
B) Concentration colorized gradient of Fe^{2+} (D) diffusion for finalized design geometry at T = 100 days
C) Concentration plot in Moles of Fe^{3+} vs. time at opposite corners of the reactor model (blue/green dots)
D) Concentration plot in Moles of Fe^{2+} vs. time at opposite corners of the reactor model (blue/green dots)

As shown in Figure 21 above, the concentration of each redox shuttle varies in each compartment and is not symmetrical due to the geometry. Because the reaction rate in the model is volume dependent, the greater volume of the O_2 compartment results in greater production of

Fe^{3+} in the system than Fe^{2+}, and consequently consumes more Fe^{2+} than Fe^{3+}. This imbalance is highlighted below in Figure 22, which shows the long-term steady state of this imbalance in the model.

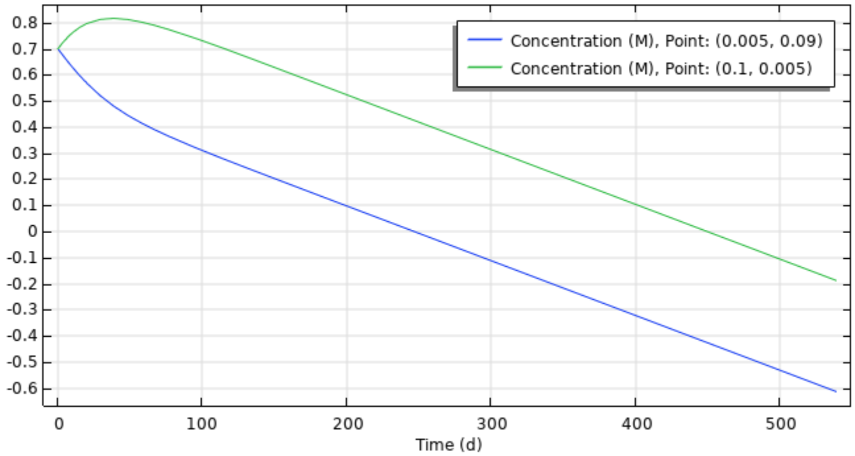


Figure 22. COMSOL plot of redox Fe^{2+} shuttle concentration vs time, showing Fe^{2+} consumed at Day 240

This imbalance is due only to the nature of modeling the reaction of $Fe^{3+} \rightarrow Fe^{2+}$ and $Fe^{2+} \rightarrow Fe^{3+}$ on a per volume basis, which may be slightly different than the actual reaction's behavior. In addition, this consumption of Fe^{2+} would only first happen ~240 days after startup and would be at the very top of the O_2 compartment (blue dot in Fig. 21). As time progressed, other areas of the O_2 compartment would consume their local amount of Fe^{2+} if not refilled. With proper chemical concentrations of redox shuttles and photocatalysts, the reaction rates and steady state concentrations can be readily controlled given sufficient chemical engineering. At a minimum, servicing the reactors at least twice a year to rebalance their concentrations of redox shuttles and photocatalysts would be necessary (given Fe^{2+} would start to be consumed in the first 240 days). At most, additional chemical control features and redox & photocatalyst refill lines could be used to accurately control the amount of each solute in each solution compartment on a much smaller time scale. Further research is needed to determine how desirable this may be, and if such additional features provide a production benefit at a reasonable cost. Overall, the system does work as intended, and clearly demonstrates sufficient transport rate to facilitate production of H_2.

Finalized Structural Analysis

The results of the FEA of the finalized design are similar to the previous designs, shown in Fig 23, simulating gravity forces on the structure and hydrostatic pressure along the insides of the tanks. The stresses are greater at the bottom portion of the outer walls of the design. The taller compartment, which would generate O_2, having the greatest stresses. The stresses are larger than previous designs by around a factor of ten. This is due to the increase in hydrostatic pressure due to an increase in the peak height of the water in the O_2 compartment in the design. FEA was conducted for five materials: HDPE, LDPE, PET, PP, & PMMA. The comparison between the max stresses and yield strength of the material can be seen in Table 2.

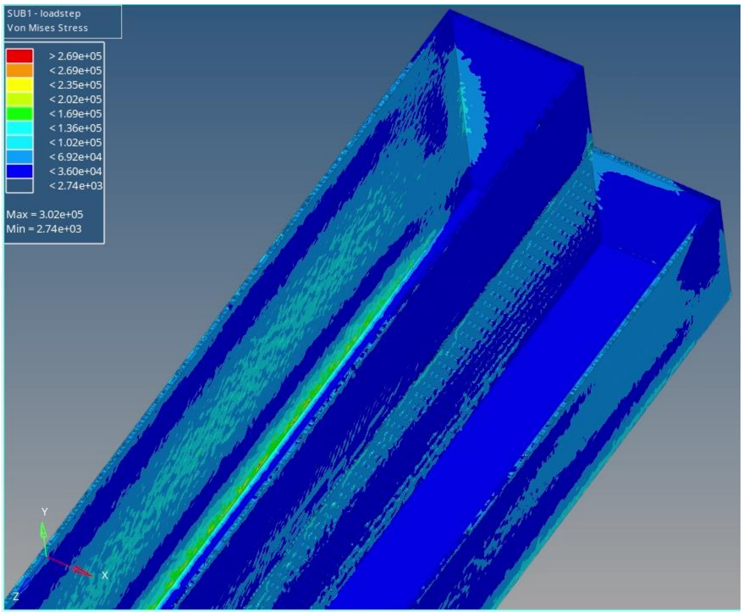


Figure 23. FEA of HDPE plastic on the Final Design. Max Von Mises Stress found to be 302 kPa

Table 2. Max Von Mises Stress and Yield Strength of Plastics for the Final Design

Material	Max Von Mises Stress	Yield Strength
HDPE	302 kPa	23.0 - 29.5 MPa
LDPE	382 kPa	7.0 - 16.0 MPa
PET	389 kPa	40 - 85.5 MPa
PP	351 kPa	31 - 45 MPa
PMMA	386 kPa	65 - 83.4 MPa

DISCUSSION / RECOMMENDATIONS

Recommendation of Design to Sponsors

Given the expectations to provide multiple options for the sponsors to consider, the team seeks to recommend one design over the others, namely the horizontal side-by-side design, which is shown above in Figure 24. The horizontal design received the highest score from the Pugh chart (Figure 9) analysis and demonstrates several strengths. One such strength is its rigid nature which ensures the reactor's dimensions do not vary in such a way that the fluid flow is affected. Chiefly, a more rigid design maintains a total diffusion length scale of 10 cm over more flexible designs, which is in accordance with the recommendations of Professor Bala Chandran's EES research paper to ensure efficient redox shuttle transport [1]. Another strength is that the scalability of this design is achieved simply by extending the length past 40 cm to accommodate a larger volume of water. There is no need to change the dimensions of the porous separator (height and width) or the height of the reactor itself, as they are chosen to conform to the recommended geometry for best redox diffusion. Lastly, the thickness of the material (2 mm) maximizes the transmission of sunlight (over 90%) while being thick enough to minimize or eliminate the need for external supports.

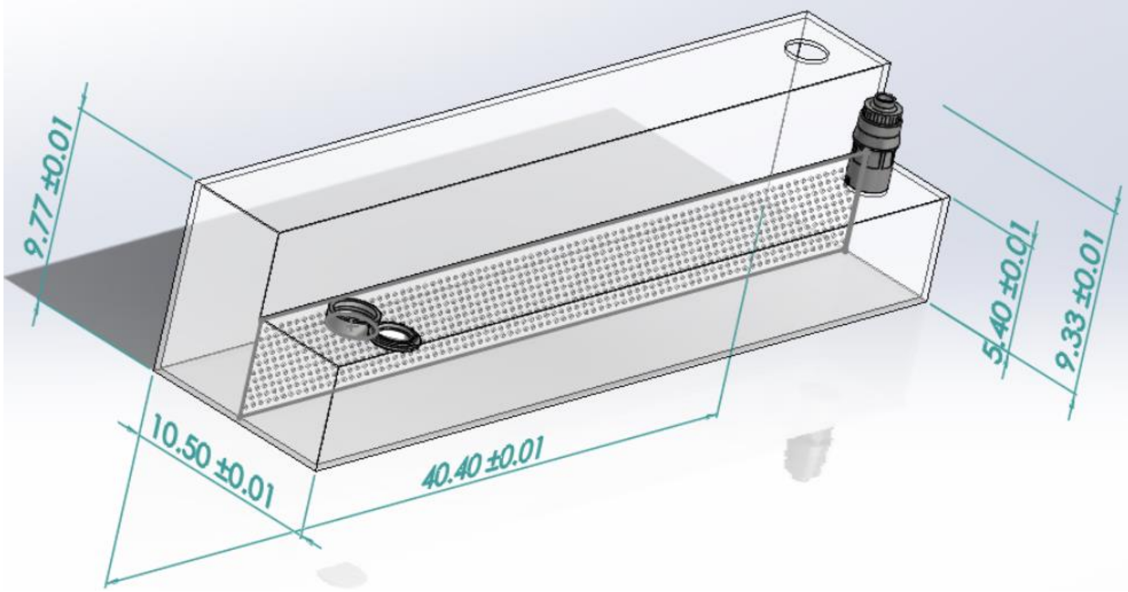


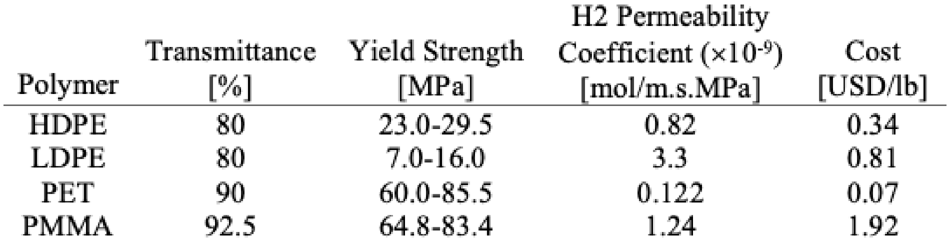
Figure 24. CAD of horizontal side-by-side design with dimensions. A float valve is shown on top of the right tank to allow for hydrogen gas to leak and be collected. Note a collection tube is not included in the CAD but is the means to transport and store hydrogen.

With strengths come weaknesses, and the team recognizes the potential pitfalls of the design. One such issue is ensuring the porous membrane material (polypropylene) remains connected with the frame to prevent leaks while ensuring fluid flow. Additionally, the rigid, non-foldable nature of the plastic reactor means it is less transportable than plastic bag style reactors, initially preferred by our sponsor. These more flexible plastic options would allow for the reactors to be rolled or packaged to take up less space and could be inflated after transport and installed in large swaths to create a larger plant of hundreds of reactors. This was not part of the given design criteria, and although desirable, flexible bags were considered to be a change implemented in later design iterations of the project. Our team believes that this initial design of a rigid, side-by-side reactor format maximizes its strengths toward fulfilling the system requirements best and is worth its weaknesses for easier manufacturability and robustness.

Material Recommendation

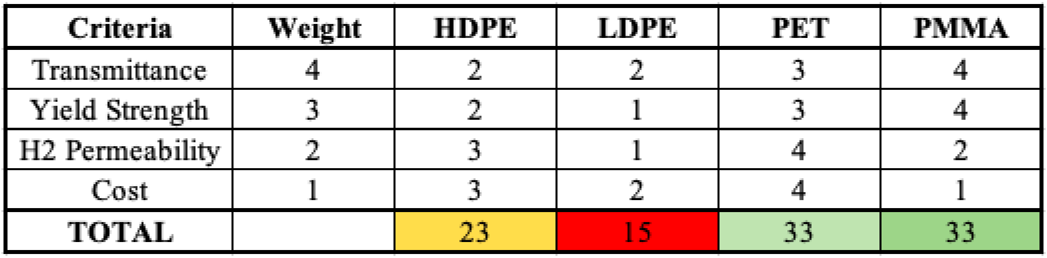
From the sponsors’ prior research as well as the team’s search, the materials for selection and evaluation include: high-density polyethylene (HDPE), low-density polyethylene (LDPE), polyethylene terephthalate (PET), and polymethyl methacrylate (PMMA), also known as acrylic. These materials have desirable high transmittance properties and yield strengths, low H_2 permeability, and low-price cost-effectiveness, as seen in Table 3.

Table 3. Polymers with their respective material properties and cost



Polymer	Transmittance [%]	Yield Strength [MPa]	H2 Permeability Coefficient ($\times 10^{-9}$) [mol/m.s.MPa]	Cost [USD/lb]
HDPE	80	23.0-29.5	0.82	0.34
LDPE	80	7.0-16.0	3.3	0.81
PET	90	60.0-85.5	0.122	0.07
PMMA	92.5	64.8-83.4	1.24	1.92

The team used this information in order to evaluate each material versus the properties listed above through a Pugh chart. The categories and corresponding weights are: transmittance (4), yield strength (3), H_2 permeability (2), and cost (1). Figure 25 visualizes the scoring and potential candidate for the reactor housing.



Criteria	Weight	HDPE	LDPE	PET	PMMA
Transmittance	4	2	2	3	4
Yield Strength	3	2	1	3	4
H2 Permeability	2	3	1	4	2
Cost	1	3	2	4	1
TOTAL		23	15	33	33

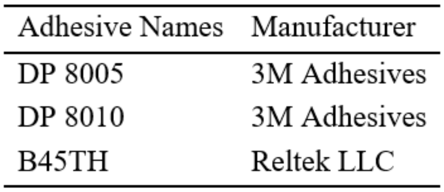
Figure 25. Pugh chart of polymers as weighted against their respective properties. As seen, PMMA and PET both scored 33, resulting in a tie. However, the team recommends PET over PMMA due to the negligible difference in cost of the overall design.

As seen in Figure 25, PMMA and PET both scored 33, resulting in a tie. However, due to the small-scale nature of the design (occupied volume of 352 cm^3 of the plastic material) the team recommends PET over PMMA. Given the volume and known densities, the cost can be calculated. PET would cost approximately \$0.075 whereas PMMA would cost \$1.75. It is the determination of the team that the difference in price between the two, as compared to the cost of the heat gun (\$649), float valve (\$39.01), and adhesive (\$38.02), is negligible. PMMA would maximize light transmitted and provide maximal structural integrity, while also maintaining a relatively low level of H_2 loss due to permeability.

Manufacturing Recommendations

There are multiple ways to manufacture the tank structure for Design 1. Some of the manufacturing techniques that we could potentially use are blow molding, injection molding, and/or a collection of welding processes. Although blow molding and injection molding would make manufacturing Design 1 simple and easy to replicate, these processes are too expensive to be manufactured for this prototype and the scope of this project. If Design 1 proves to be valuable enough for mass production, we encourage sponsors to utilize molds after cost evaluations. After considering expenses, material, and thickness, the most inexpensive process would be hot gas welding and potentially using adhesive. The polyethylene and polypropylene panels can be purchased from McMaster-Carr or any HDPE manufacturer. The panels can be either hot welded or glued using silicon structural glue. Hot-gas welding can be performed with a hot air gun and welding rod. To weld the edges of the structure one option is to feed the HDPE rod through the gun and apply pressure on the rod as the sheet and rod are heated simultaneously. Another option would be to heat the edge of the panels and clamp them together until solid. Both options require more material than the design dimensions for heating and trimming purposes. The temperature of the gas should be at 575°F for a round nozzle for welding HDPE [5]. The American Welding Society has recommended hot gas welding conditions, shown in Fig A.2. We recommend the hot gas welding method because it would generally provide a more sound structure than an adhesive method, however this method is more expensive and tedious than an adhesive method due to a low surface energy. Two-part epoxy and acrylic systems have proven to be effective adhesives. Suggested adhesives are shown in Table 4 [5]. Lap shear strength values of greater than 1,000 psi have been achieved for each of these suggestions [5]. Since these suggestions have a high tolerance for pressure, the float valve can be glued to the top panel using one of the adhesives in Table 4. These adhesives are waterproof, leak-free and have negligible change to the pH value of the overall system. The vent and hole for the float valve in the top panel can be cut with a water jet or mill.

Table 4. Approved adhesives for HDPE



Adhesive Names	Manufacturer
DP 8005	3M Adhesives
DP 8010	3M Adhesives
B45TH	Reltek LLC

Economic Analysis & Recommendation

There are several economic aspects of the design that warrant a discussion and recommendation for future use. As mentioned, some of the major costs include the float value and adhesive, along with the cost of plastic material. Given that plastics are common in industry and are inexpensive, it has little to no weight on the economic decisions. When totaling the cost of the float valve and adhesive, the result is approximately $78.89 per reactor. This in essence means that for every reactor, there is a fixed cost of that amount. However, what is significant and has not been addressed is the effect of the heat gun on the economic analysis and recommendation.

The heat gun used in this design is used for manufacturing purposes. The cost of it is about $649 which will be considered a capital expenditure, or initial investment. In order to minimize its impact on the overall cost over time, the team recommends using it as much as possible. The relationship between the cost of the heat gun and the amount of reactors made is inversely proportional, meaning the more reactors the team makes, the lower the cost of the heat gun in perpetuity. Thus, the team recommends a high production rate of the reactor in order to minimize its effect while also considering the material costs for each reactor.

Minimum Membrane Ratio Recommendation

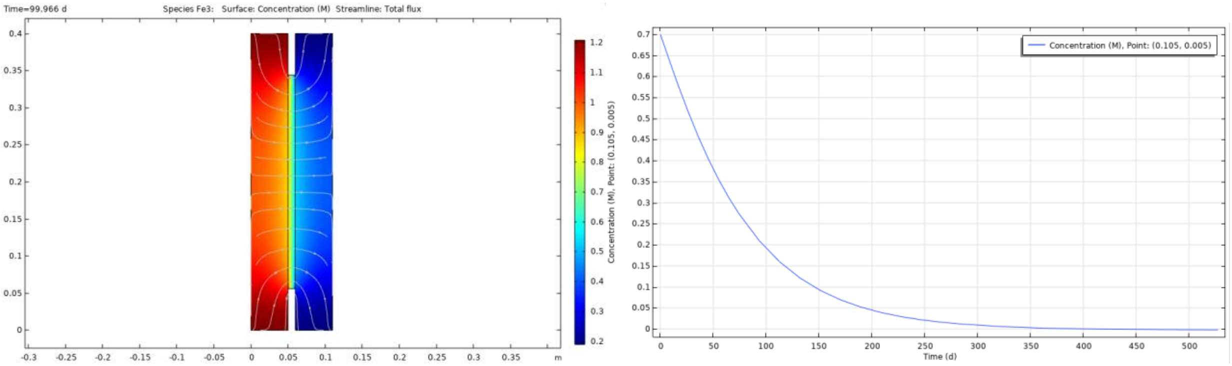


Figure 26. Graphic and plot of change in concentration for a 1:1.389 or 72% membrane to unit cell width

Based on further testing in COMSOL using the Design 1 base model, it was determined that the minimum membrane ratio that would still - though barely - facilitate hydrogen production at some measurable steady state concentration of reactants was a 1:1.389 membrane to unit cell width ratio, or 72% of the unit cell's width connected to the porous membrane. As Figure 26 above shows, the steady state concentration of redox shuttles has an effective asymptote of 0M, meaning any membrane larger than 72% will have some amount of redox shuttles at steady state operation that are never used up. To what extent this minimum of around 0M constitutes self-sustaining redox reactions is questionable, and for maximum transportability of redox shuttles the best recommendation is to have a 1:1 ratio of membrane to unit cell. Still, it is of interest to our sponsors to determine the absolute minimum ratio that would still allow for reactor operation.

Something to note is that the initial minimum ratio testing for the first 100 days of operation yielded a 1:4 ratio, or 25% membrane to unit cell. However, extending out the simulated operation time to over 1500 days shows that clearly the 1:4 ratio does not reach steady state operation within the first 100 days, rather it continues past 0M and decreases to a steady state of nearly -3M by day 1500, resulting in a stalled reaction and consumption of redox shuttles back on the 98th day. This is important to note as this is a change from the results discussed at the last meeting with the sponsors.

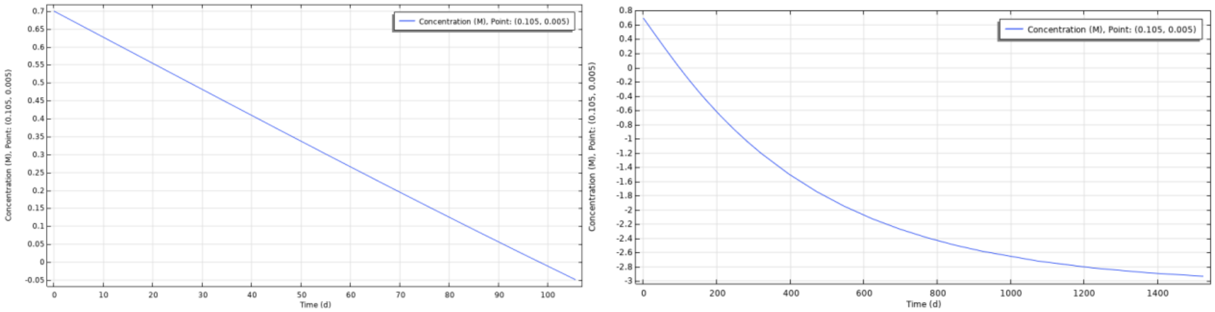


Figure 27. Plot of 1:4 membrane to unit cell width ratio operating for 100 days (left) and 1500 days (right)

A graph of the concentrations of all of the tested ratios is given in Figure 28 for reference.

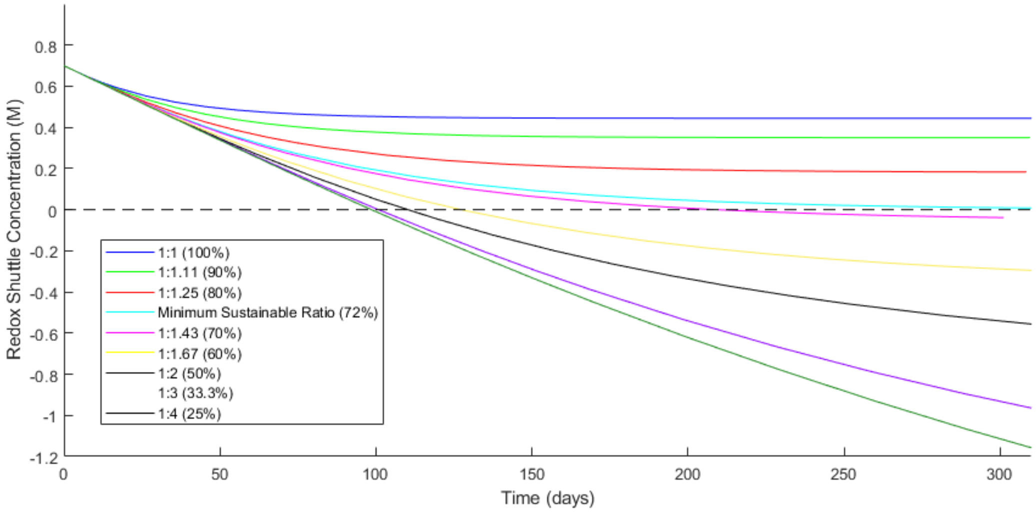


Figure 28. Plot of concentration decline for various membrane to unit cell width ratios tested in COMSOL

Additionally, the effect of breaking up the membrane into smaller, more equally spaced regions for a given membrane to unit cell ratio was also studied. Using the minimum steady state ratio of 1:1.389 (72%), it was found that increasing the number of membrane regions allowed for less decline of concentration of redox reactants, as shown in Figure 29 below.

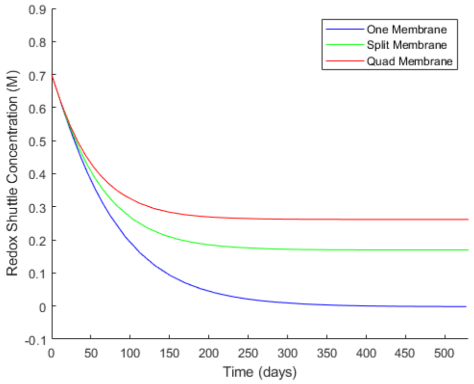


Figure 29. Plot of concentration decline for various number of membranes tested in COMSOL

CONCLUSION

In this capstone design project, we set out to design a plastic reactor for solar-hydrogen production. This task has been achieved. The reactor facilitates chemical reactions, using solar energy as fuel, and soluble redox shuttles for electron transport, to break apart water in hydrogen and oxygen byproducts. The design minimizes light absorption by the plastic tank housing by utilizing PET material and minimizes time for rapid redox shuttle transport. The recommendation of the team is to have a membrane to unit cell ratio of 72% or greater to ensure sufficient redox shuttle transport for steady state operation. The safe operation of the reactor of minimizing the mixing of hydrogen and oxygen products is carried out by the utilization of two compartments. Without the need for a pump, this design minimizes energy consumption by the reactor components, and allows for scaling of the reactor to different sized volumes of water due to its geometry.

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ACKNOWLEDGEMENTS

We would like to thank our sponsors, Professor Bala Chandran and Professor Ardo, as well as graduate student Zeijie Chen, for their support and guidance throughout the project, as well as our supervising advisors Professor Saitou and Professor Cooper for their assistance and support to our team throughout the project.

SOURCES

[1] Bala Chandran, R. , Breen, S. *et al.* Evaluating particle-suspension reactor designs for Z-scheme solar water splitting via transport and kinetic modeling. *Energy Environ. Sci*., 11, 14, 115. (2018).

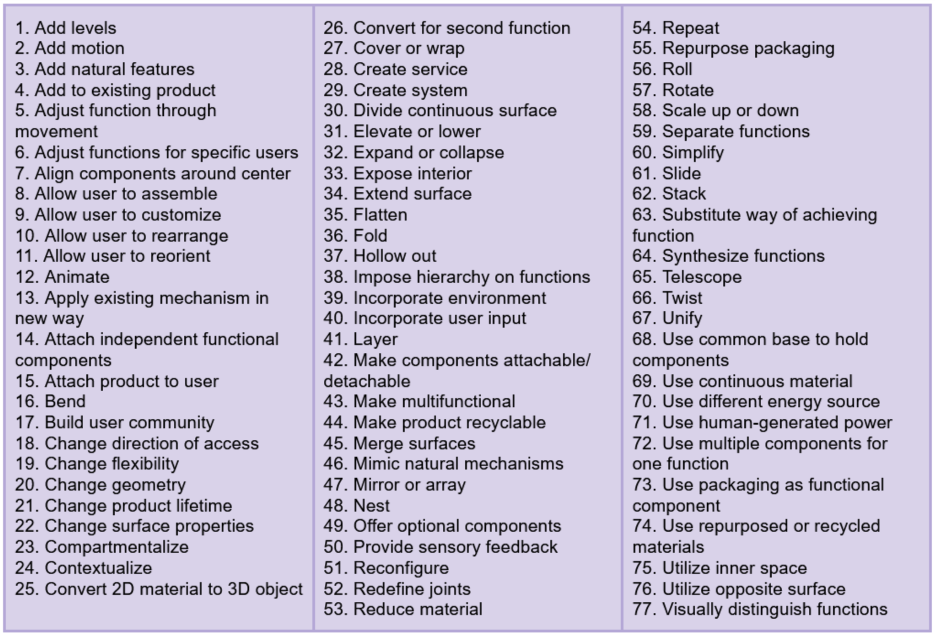
[2] Shastik, E., Romanova, A., Laurinavichene, T. *et al.* Plastic bags as simple photobioreactors for cyanobacterial hydrogen production outdoors in Moscow region. *Int J Energy Environ Eng* 11, 1–8 (2020).

[3] James, Brian D., George N. Baum, Julie Perez, and Kevin N. Baum. Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production. 2009.

[4] Jacobsson, T. Jesper. Photoelectrochemical water splitting: an idea heading towards obsolescence? *Energy Environ* 11, 1977-1979 (2018).

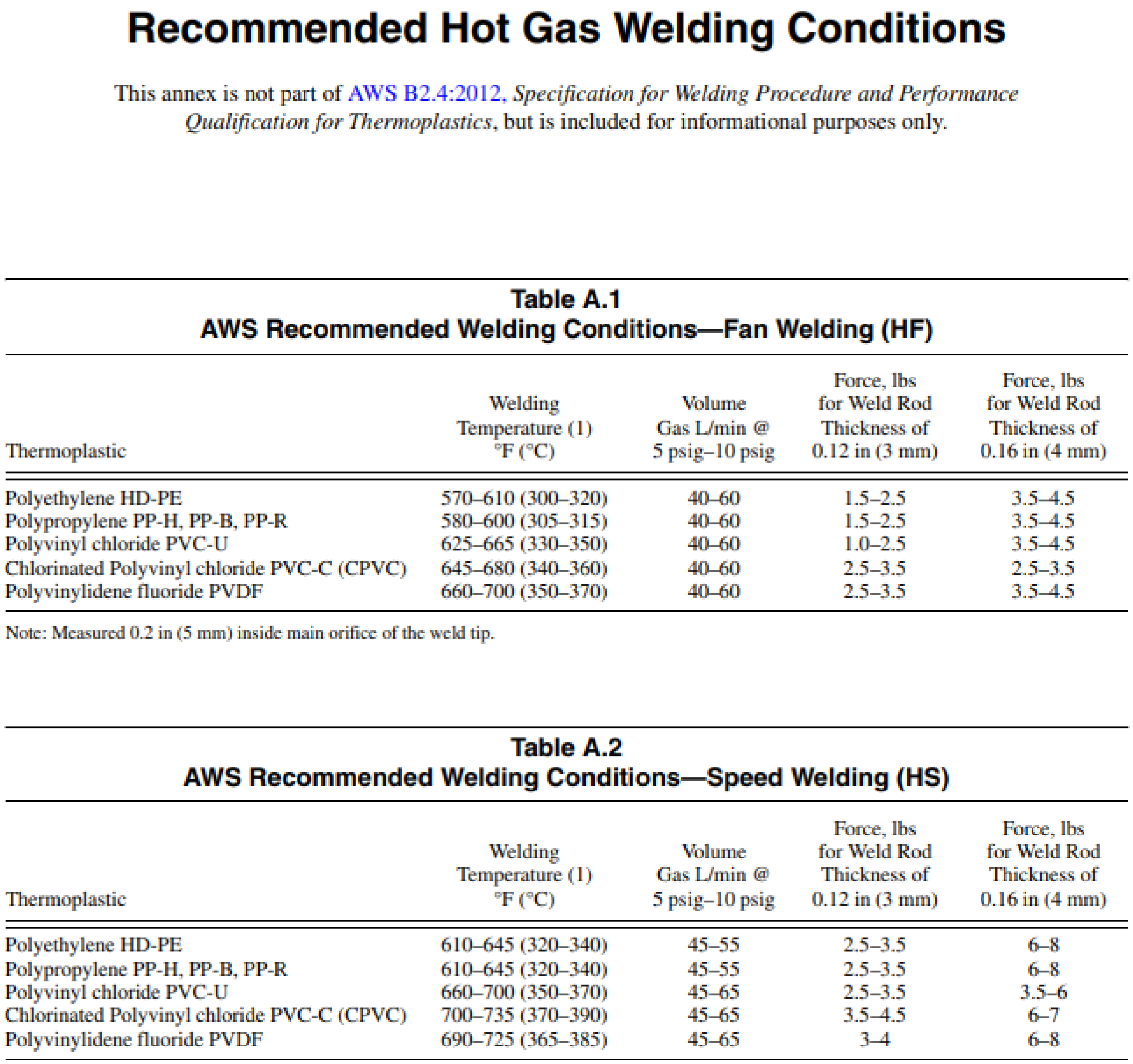
[5] Vycom. HDPE Fabrication Guide.Vycom PVC Solutions (2013).

Appendix



1. Add levels
2. Add motion
3. Add natural features
4. Add to existing product
5. Adjust function through movement
6. Adjust functions for specific users
7. Align components around center
8. Allow user to assemble
9. Allow user to customize
10. Allow user to rearrange
11. Allow user to reorient
12. Animate
13. Apply existing mechanism in new way
14. Attach independent functional components
15. Attach product to user
16. Bend
17. Build user community
18. Change direction of access
19. Change flexibility
20. Change geometry
21. Change product lifetime
22. Change surface properties
23. Compartmentalize
24. Contextualize
25. Convert 2D material to 3D object
26. Convert for second function
27. Cover or wrap
28. Create service
29. Create system
30. Divide continuous surface
31. Elevate or lower
32. Expand or collapse
33. Expose interior
34. Extend surface
35. Flatten
36. Fold
37. Hollow out
38. Impose hierarchy on functions
39. Incorporate environment
40. Incorporate user input
41. Layer
42. Make components attachable/ detachable
43. Make multifunctional
44. Make product recyclable
45. Merge surfaces
46. Mimic natural mechanisms
47. Mirror or array
48. Nest
49. Offer optional components
50. Provide sensory feedback
51. Reconfigure
52. Redefine joints
53. Reduce material
54. Repeat
55. Repurpose packaging
56. Roll
57. Rotate
58. Scale up or down
59. Separate functions
60. Simplify
61. Slide
62. Stack
63. Substitute way of achieving function
64. Synthesize functions
65. Telescope
66. Twist
67. Unify
68. Use common base to hold components
69. Use continuous material
70. Use different energy source
71. Use human-generated power
72. Use multiple components for one function
73. Use packaging as functional component
74. Use repurposed or recycled materials
75. Utilize inner space
76. Utilize opposite surface
77. Visually distinguish functions

Figure A.1. Design heuristics as provided from the concept generation learning block.



Recommended Hot Gas Welding Conditions

This annex is not part of AWS B2.4:2012, *Specification for Welding Procedure and Performance Qualification for Thermoplastics*, but is included for informational purposes only.

Table A.1
AWS Recommended Welding Conditions—Fan Welding (HF)

Thermoplastic	Welding Temperature (1) °F (°C)	Volume Gas L/min @ 5 psig–10 psig	Force, lbs for Weld Rod Thickness of 0.12 in (3 mm)	Force, lbs for Weld Rod Thickness of 0.16 in (4 mm)
Polyethylene HD-PE	570–610 (300–320)	40–60	1.5–2.5	3.5–4.5
Polypropylene PP-H, PP-B, PP-R	580–600 (305–315)	40–60	1.5–2.5	3.5–4.5
Polyvinyl chloride PVC-U	625–665 (330–350)	40–60	1.0–2.5	3.5–4.5
Chlorinated Polyvinyl chloride PVC-C (CPVC)	645–680 (340–360)	40–60	2.5–3.5	2.5–3.5
Polyvinylidene fluoride PVDF	660–700 (350–370)	40–60	2.5–3.5	3.5–4.5

Note: Measured 0.2 in (5 mm) inside main orifice of the weld tip.

Table A.2
AWS Recommended Welding Conditions—Speed Welding (HS)

Thermoplastic	Welding Temperature (1) °F (°C)	Volume Gas L/min @ 5 psig–10 psig	Force, lbs for Weld Rod Thickness of 0.12 in (3 mm)	Force, lbs for Weld Rod Thickness of 0.16 in (4 mm)
Polyethylene HD-PE	610–645 (320–340)	45–55	2.5–3.5	6–8
Polypropylene PP-H, PP-B, PP-R	610–645 (320–340)	45–55	2.5–3.5	6–8
Polyvinyl chloride PVC-U	660–700 (350–370)	45–65	2.5–3.5	3.5–6
Chlorinated Polyvinyl chloride PVC-C (CPVC)	700–735 (370–390)	45–65	3.5–4.5	6–7
Polyvinylidene fluoride PVDF	690–725 (365–385)	45–65	3–4	6–8

Figure A.2. American Welding Society B2.4 - Recommended Hot Gas Welding Conditions for various plastics.

ME 450 Supplemental Appendix

Engineering Standards

Although the team did not specifically use standards, one that is of concern is the engineering standard ISO 10156:2017 for determining whether or not a gas or gas mixture is flammable in air and whether a gas or gas mixture is more or less oxidizing than air under atmospheric conditions. This establishes the methodology for testing flammability limits using specific apparatuses, namely in the determination of flammability limits of gas mixtures containing flammable and inert gases and air. Moreover, in terms of hydrogen safety, which is important for the scope of this project must be stated clearly as it dictates the limits at which the reactor can operate. The flammability limits based on the volume percent of hydrogen in air at 1 atm are 4.0 and 75.0. The flammability limits based on the volume percent of hydrogen in oxygen at the same pressure are 4.0 and 94.0. This information in tandem with the engineering standard ISO 10156 provides an established and well-informed decision by the team to ultimately create a two-compartment reactor in order to reduce the probability of such hazardous mixing occurring.

Engineering Inclusivity

The structural design and analysis of plastic component reactors does not have an impact on social identities to our knowledge. However, there was an interesting power framework within this project. As students, we represent undergraduate mechanical engineers who actively interacted with Ph.D. chemical engineers with years of lab experience during our stakeholder engagement process. Their level of education and age are important in understanding both hidden and invisible expressions of influence in this project. When we initially began this project, we were excited to tackle problems that could change hydrogen production forever. The sponsors were also eager to have young, fresh minds look at some of their work and come up with groundbreaking ideas. Unfortunately, this was not the case for both parties. As undergraduate mechanical engineers, we initially found it difficult to provide new concepts to a chemical engineering problem besides manufacturing and design which was a result of the universities and stakeholders' hidden power. However, we knew that our knowledge of structural supports would be very useful to our stakeholders/sponsor and eventually determine our final design. Initially there were some disagreements with our horizontal compartment choice. In our opinion, the horizontal design was structurally more sound and ensured the balance of redox shuttles better than the sponsor's vertical preference. The sponsors became more open to our design decision once we incorporated the vertical design into our presentations and analysis, which was our invisible power. We quickly realized that we must be completely inclusive with all preferred designs with analysis before we can steer stakeholders in a different direction.

Although this project contributes mostly to science and has no need for a socially inclusive design, there are some global inclusivity issues that could have been addressed. As a result of the time it took to understand the project and create an accurate COMSOL model, we did not have time to address global sustainability issues. If our prototype will be used at a higher scale than what we anticipated, life cycle analysis must be addressed.

Environmental Context Assessment

The reactor makes significant progress towards creating a new reliable source of renewable energy, which will lower the impact on the environment from human energy consumption. The production of hydrogen can be used for the fuel of hydrogen fuel cells. Hydrogen fuel cells have many applications, including transportation and stationary, portable, and emergency backup power applications, and can replace less environmentally friendly alternatives like combustion engines. Hydrogen fuel cells do not produce any harmful emissions, only emitting water. A significant issue is the costs associated with producing the hydrogen that is used in hydrogen fuel cells. Having a reactor that can cheaply produce hydrogen will be a significant factor in the economic success and sustainability of hydrogen fuel cells.

The reactor should not have any undesirable consequences to the environment other than from its use of plastic. The plastic is multi-use and disposal is easier to control compared to plastics used commercially. The water that is supplied for the production of hydrogen is eventually emitted from the use of hydrogen fuel cells, which should have negligible effects on the environment.

Social Context Assessment

Some of the key questions about the future of sunlight-driven hydrogen reactors revolve around their cost and efficiency. To be able to be economically competitive, passive sunlight reactors must produce a comparable amount of hydrogen at close to even or better cost per kilogram than hydrogen produced from fossil fuels. Current estimates for hydrogen production from natural gas range in the $1.25 to $3.50 range per kilogram, and our first design iteration of solar reactor is based on a 10% maximum theoretical efficiency, with realistic estimates of 1% solar to hydrogen (STH) conversion efficiency. For our $79 unit, the resulting comparable cost is $44.50 per kilogram of hydrogen - assuming 0.2425 M or 0.485 g of H_2 per day operating for 10 years at max theoretical efficiency. These reactors at this current efficiency and stage of development are not market ready, much less ready for large-scale usage. With necessary development and production, the ability to produce hydrogen sustainably and economically - without the use of fossil fuels - can be the next big advancement in circular clean energy. Though not the most commonly used fuel, hydrogen gas and hydrogen fuel cell technologies are a proven path to an energy cycle that does not involve greenhouse gases, making it a nearly 100% renewable energy source. Provided that hydrogen is readily produced sustainably using solar reactors, this form of fuel can lead to growth in sustainable fuels and uses that can supplant the current dependency on many fossil fuel types for most production processes, from plastics to metals. Current trends of hydrogen fuel cell vehicles will also play a role in hydrogen fuel powering various forms of transportation. Though rather safe in its current state, future advances in safely storing and using hydrogen fuel will be needed as its use in other forms of transport and energy consumption increase. In the short term, this passive technology will be a trade-off means of producing hydrogen and will pave the way for more investment in developing the generation and usage of hydrogen fuel and its associated technologies. As our sponsors have reminded us, the potential benefits of sustainably produced hydrogen can revolutionize the way we use energy and play a significant role in a world with green energy that has little to no carbon footprint. If the technology succeeds, it will greatly benefit our planet, and hopefully our society as well. Adoption of hydrogen as a fuel source will be highly dependent on solving questions of efficiency - for both production and consumption - as well as storage and transportation. Given the massive and established infrastructure already in place for natural gas - our current short term main fuel source - hydrogen gas and hydrogen fuel have an easy path for adoption, as well as adjustments for shortages. The main issue to tackle will be consistent production to meet necessary demand should the entire energy economy be based on hydrogen alone. Given this unlikely avenue, it is much more likely that hydrogen will play a role amongst a host of other renewable fuel sources, as well as renewable electricity generated through wind and solar.

Ethical Decision Making

A discussion regarding the ethics and ethical decision making for this project is justified. Some of the ethical issues that the team faced this semester include, but are not limited to: balancing sponsors' needs/desires with the requirements of the course, dealing with a teammate's absence, and ensuring that the team fully addressed the concerns of the sponsors. A difficulty the team experienced early was the ambitious goals set forth by the sponsors, moreover, understanding our own capabilities and limitations. Unfortunately, it took a month before the team knew that there were several aspects of the project we would be unable to achieve, such as complex simulations of the flow analysis via COMSOL. Additionally, the team was faced with losing a team member midway through the project. The team did not know how to properly respond nor addressed it with said member after he left. This inhibited the collective's ability to finish the project fully, ahead of schedule or on time. Excuses should not be made about lack of transparency with the sponsors or professors, but no team member knew how to deal with this. However, much has been learned about it since. Lastly, there was a moment towards the end of the semester when the team was faced with academic challenges due to course loads and gravitated towards settling on suboptimal performance. While the team understood that morale was low, this does not grant us the opportunity to accept less than our highest potential. Ultimately the team was able to move past this together and was content with the performance afterwards. Ethically, these challenges were unique to this team but showed us the need to maintain integrity, admit fault when warranted, and exceed our expectations for the betterment of the sponsors and project overall.