Suggested Design Projects – 2023-2024

1. Biohybrid CO_2 Electrolysis for the Direct Synthesis of Polyesters (Recommended by Leonard Fabiano, Adjunct Professor, Penn)

Background

A great deal of research has been conducted over the past decade or more to achieve a sustainable CO_2 cycle. Electrolysis of CO_2 has been studied extensively but the products have been limited to C-1 through C-3 products. The references report the integration of CO_2 electrolysis with microbial fermentation to directly produce poly-3-hydroxybutyrate (PHB).

The biohybrid system comprises the electrochemical conversion of CO_2 to formate on Sn catalysts deposited on a gas diffusion electrode and subsequent conversion to PHB by Cupriavidus nectar cells in a fermenter. The researchers believe that strategies will be useful for establishing other biohybrid systems to produce other chemicals.

Problem Statement

Here is the scenario for your company/project: BIOCHEMTECH, Inc., your company, has developed a partnership with the research team that produced the results described in the first reference. They see that this work may be a breakthrough and further development may open up a serious new focus on other chemicals. Your team is part of the Process Engineering and Development Group that performs early evaluation of new technologies.

Your goal is to prepare a process design for a 100 million pound per year facility to produce PHB. It is recognized that all questions of viability may not be answered presently. Your team is to make that judgement. Major assumptions will need to be made. Your team must identify if there are any areas of technology weakness and speak to the quality and sufficiency of the data presented. These will become front and center as the detailed design is developed.

Your company expects to use your results to decide to recommend further research goals and development needs that would be shared with the research team from the Department of Chemical and Biomolecular Department, Korea Advanced Institute of Science and Technology, Daejon, 34141, South Korea.

To that end, part of your work is to decide on research targets to provide to KAIST that will result in an economically attractive design. For example, you may recommend specific technical improvements in the gas electrolysis step (electrode design, allowable concentration of formate in the buffer, etc.), the biological transformation (often expressed in terms of rate, titer or yield), or the downstream separations/purification - or any combination of these or other areas of the technology. It is strongly recommended that your models of the process (mass and energy balances, equipment sizing and economics) consider that you may want to adjust any of several input variables and have everything recalculated automatically, for ease of sensitivity analysis to determine where KAIST should focus their research efforts. Your report should show "current state" and "research target" design and economics.

The benchmark for economic success is 15 % IRR. The plan would be to expect the facility to be built in the USA in an existing Gulf Coast location. Utilities available will be typical for the location.

References

J. Lim et. al., Proceedings of the National Academy of Sciences, 2023, Vol 120, No. 14, Biohybrid CO_2 Electrolysis for the Direct Synthesis of Polyesters from CO_2 (https://doi.org/10.1073/pnas.2221438120)

Chemical Engineering Progress, Early Research Proves Synthesizing Polyester from CO_2 is Possible, May 2023, pp. 9-10

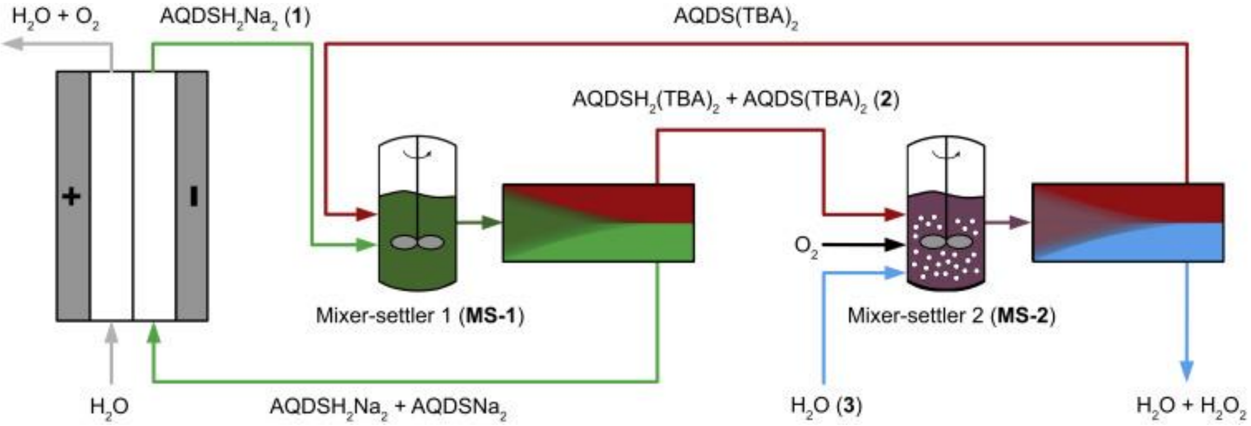
2. A Greener Route to Hydrogen Peroxide
(Recommended by Gary Sawyer, Process Evaluations LLC)

Aqueous hydrogen peroxide has applications from household antiseptic to paper bleaching to chemical intermediates such as in the production of propylene oxide.

The legacy process to make hydrogen peroxide is the anthraquinone (AQ) process, which feeds hydrogen and oxygen to an organic "working solution", from which the hydrogen peroxide is extracted into water.[1] Large scale hydrogen production by steam methane reforming (SMR) is widely commercialized but is a significant contributor to greenhouse gas emissions.[2]

Both hydrogen and oxygen can be made from electrolysis of water, but either excess hydrogen is generated, or supplemental oxygen is needed, since $H_2O \rightarrow H_2 + \frac{1}{2} O_2$, and we need equimolar hydrogen and oxygen. **Part 1 of your project** is to calculate the electricity consumption per pound of hydrogen peroxide, assuming water electrolysis with excess hydrogen generation. Your group is responsible for researching electricity consumption for water electrolysis. Calculate the cost of electricity used for this process, using historical pricing data from www.eia.gov. However, no process design, capital or operating costs are required for the AQ or electrolysis processes.

A review of direct synthesis routes for hydrogen peroxide is found in reference 1 below. **Part 2 of your project** focuses on a novel electrochemical route by Murray, et. al. [3], as shown below.



The reference article has performance data on faradic efficiency (how many electrons – or current needed) and voltage to produce hydrogen peroxide. Power consumption is calculated from P=I x V, where P is power in Watts, I is amperage, and V is volts. Note that there are now two loops of "working solution". Your project is to prepare a more detailed material balance and process flow diagram, and calculate equipment sizes, needed to produce 100,000 metric tonnes per year of H_2O_2 contained in as a 35 wt% solution in water, a commercially common concentration. The bulk of your effort and report will be

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[1] https://www.google.com/url?sa=i&rct=j&q=&esrc=s&source=web&cd=&cad=rja&uact=8&ved=0CAQQw7AJahcKEwiY5e_c4f35AhUAAAAAHQAAAAAQAg&url=https%3A%2F%2Fwww.mdpi.com%2F2073-4344%2F8%2F9%2F379%2Fpdf&psig=AOvVaw2IB0ygXoyV4HzV46yVppk5&ust=1662470989574872

[2] 9 kg CO2 / kg H2, per Argonne GREET Publication : Updates of Hydrogen Production from SMR Process in GREET® 2019 (anl.gov)

[3] Electrosynthesis of Hydrogen Peroxide by Phase-Transfer Catalysis: Joule (cell.com)

on this process. Full capital and operating costs and profitability analysis should be included, to determine the economic viability of this process.

Part 3 of your project is to compare greenhouse gas emissions of the three routes to determine whether there are societal benefits, independent of the economics, to the electrosynthesis of hydrogen peroxide –

- Conventional AQ using hydrogen from SMR
- Conventional AQ using hydrogen from electrolysis
- Electrosynthesis of hydrogen peroxide in Part 2 of your project.

If needed, you will be given references for greenhouse gas emission rates for electricity from various sources as well as that of pure oxygen, required for the AQ process.

3. Lithium Extraction from Oil Field Brine
(Recommended by Rick Bockrath, Consultant – retired from DuPont)

Background

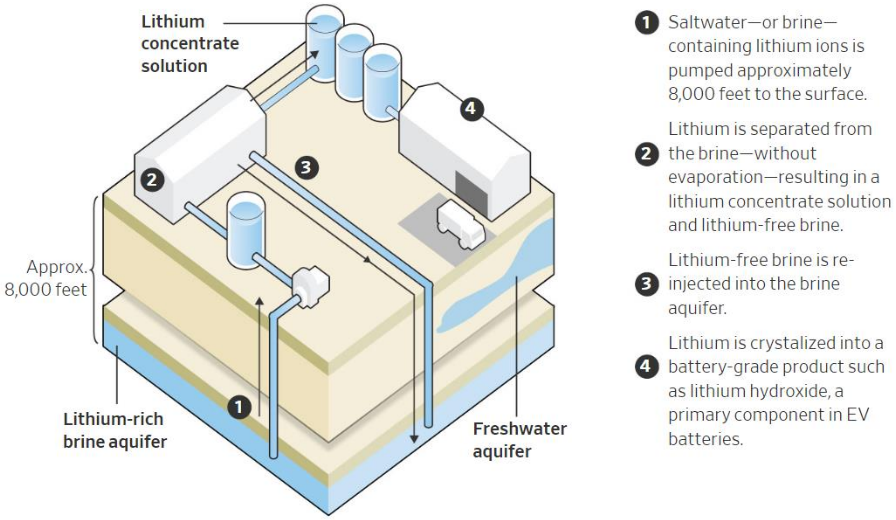
It is clear that the world is in rapid transition from gas powered to EV based autos. The speed of the transition will be heavily impacted by the rate at which the supply chains for key materials are markedly increased. As an example, it is estimated that lithium supply must increase by a factor of 10 to 18 by 2050 depending on the rate of adoption of EVs.

Problem Statement

You are a Senior Vice- President of Sourcing for a major automobile company. Sourcing of lithium has become a major headache in both the near and long term. Current lithium pricing is a factor of 6 higher than late 2020 pricing. In late 2022 pricing reached a factor of 12 before “falling” to “only” a factor of 6. The only way for pricing to drop further is to increase supply faster than demand. This means you can’t afford to ignore any potential technology or lithium sourcing options.

One source that is getting traction is direct lithium extraction from oil field brines.

Direct lithium extraction



① Saltwater—or brine—containing lithium ions is pumped approximately 8,000 feet to the surface.

② Lithium is separated from the brine—without evaporation—resulting in a lithium concentrate solution and lithium-free brine.

③ Lithium-free brine is re-injected into the brine aquifer.

④ Lithium is crystalized into a battery-grade product such as lithium hydroxide, a primary component in EV batteries.

Source: E3 Lithium

There are multiple start-up companies involved in this technology development. While you are nervous about connecting your EV future to supply of lithium from oil field brine, you can’t afford to ignore this source. A “back of the envelope” calculation indicates that the yearly supply of lithium from this source probably exceeds the world’s current lithium production.

Before talking to any of these companies, you want an internal evaluation of the technology. Since this technology is in the early stages of development, a number of optimistic assumptions will need to be made. If the results generate promising economics, then your company will approach the start-ups. If the results are negative, then you will focus on other options. An IRR greater than 20% should be sufficient. Assume a 20,000 metric ton/year plant size.

You have created a Scientific Advisory Board to help define a number of the key assumptions you will need for the study.

- The technology source is E3 Lithium. The key patent to use in your analysis is WO 2021/119841 A1. This application provides information on absorption material composition, means of preparation and efficiency in use. The material seems highly selective to Li extraction from a complex brine matrix.
- E3 Lithium is focused on Alberta brine which is low in lithium (70 mg/liter). Your focus is on Permian Basin brine. For this study assume the lithium level is 250 mg/liter. Other references indicate that Argentinian and Arkansas brines are more like 500+ mg/liter so this seems reasonable.
- Assume the absorption material can remove the lithium down to a level of 20 mg/liter at a loading of 3 wt%
- The preferred desorption agent is ammonium persulfate. This is the only agent that did not appear to attack the absorption material (selective manganese loss). Ammonium persulfate is a redox agent and it is believed that this redox potential dramatically lowers manganese losses versus the other non-redox agents tested (hydrochloric and sulfuric acid).
- The moles of ammonium persulfate used is ~ 4 moles per mole of lithium extracted in the patent examples. The Board believes that the persulfate is probably being used to adjust the pH to the preferred 8.0 as well as being a redox agent in the patent examples. It is too expensive to use as a pH adjustment agent commercially. It is proposed that the amount of ammonium persulfate to use is one mole to one mole of manganese released into the lithium extractant if sulfuric acid is the agent. Sulfuric acid is to be used for pH adjustment.
- The Board recommends you review a recent Lilac Solutions US patent (10,505,178 B2) which gives a very good grounding on absorber/desorber methodologies and equipment choices.
- The absorption material composition and means of manufacture must be determined by your team based on the E3 WO patent and you should cost it using the following tool. The tool includes metal recovery if justified.

https://catcost.chemcatbio.org/

- Assume a material bed life of 6 months.
- The lithium extracted is not pure enough to be used directly in EV batteries. The various start-up companies have all partnered with firms who handle the final purification and battery creation. For the purposes of this study assume that the downstream partner will charge $20/lb for final purification. You will be supplying the crude to them as a solid prill. As you develop your flowsheets and expected purity profile, you will need to review this with the Board to ensure alignment on expectations from the DLE step.
- The full plant would include the brine recovery system, extractors, solid formation area and depleted brine reinjection. The brine recovery and reinjection sections are outside of your scope. In a recent presentation by E3 Lithium (ref. 3), CAPEX information was given for these sections. Their project is designed for handling brines with lithium loadings of 70 mg/liter versus our expected 250 mg/liter. The CAPEX to use for the brine and reinjection sections in your study is $110 million USD. This is based on prorating the CAPEX in the E3 presentation by the ratio of 70/250 to the 0.7 power.
- You will need water for washing the lithium off of the absorption material. Since you are making a solid prill, this water can come from the dewatering stage in your process. Net water usage should be small.

General Considerations

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Make sure you fully document your assumptions in your analysis.

References

1) https://wsj-article-webview-generator-prod.sc.onservo.com/webview/WP-WSJ-0000937632?adobe_mc=TS%3D1687209238%7CMCMID%3D32280185249314078217552540345919788003%7CMCORGID%3DCB68E4BA55144CAA0A4C98A5%40AdobeOrg&wsj_native_webview=android&ace_environment=androidphone%2Cwebview&ace_config=%7B%22wsj%22%3A%7B%22djcmp%22%3A%7B%22propertyHref%22%3A%22https%3A%2F%2Fwsj.android.app%22%7D%7D%7D
2) https://seekingalpha.com/article/4468468-a-look-at-direct-lithium-extraction-dle-and-some-of-the-dle-lithium-companies
3) https://www.e3lithium.ca/investors/ Corporate Presentation

4. Post-Combustion CO_2 Capture using Desublimation Technology (Recommended by Katie Piotrzkowski, Penn)

Background

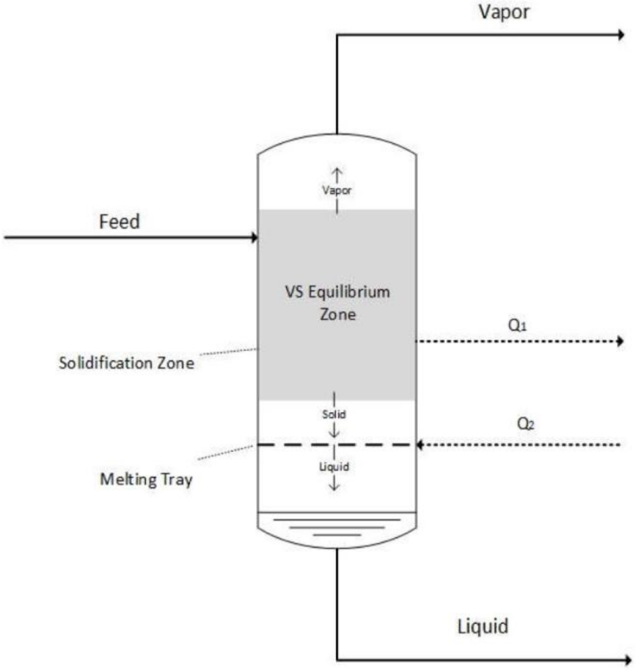
Carbon dioxide levels in the atmosphere are rapidly rising causing irreversible climate change. One of the largest contributors to carbon dioxide emissions, 25% of U.S. emissions, is burning fossil fuels for electricity at power plants. Post-combustion capture (PCC) is one method to reduce CO_2 emissions by capturing the CO_2 from the flue gas of the coal-fired power plant.

Problem Statement

There are multiple technologies in development and pilot plant testing for PCC including absorption, adsorption, and membrane processes. These technologies have proven to be effective in separating CO_2; however, each comes with certain disadvantages. Absorption has severe operational risks due to solvent degradation issues and produces potentially hazardous waste, as well as requiring a significant amount of energy to desorb CO_2 from the solvent. There are significant scaling issues with adsorption as well as high operational costs and large energy requirements due to substantial pressure changes. Membrane technology is very expensive to capture 90% of the CO_2.

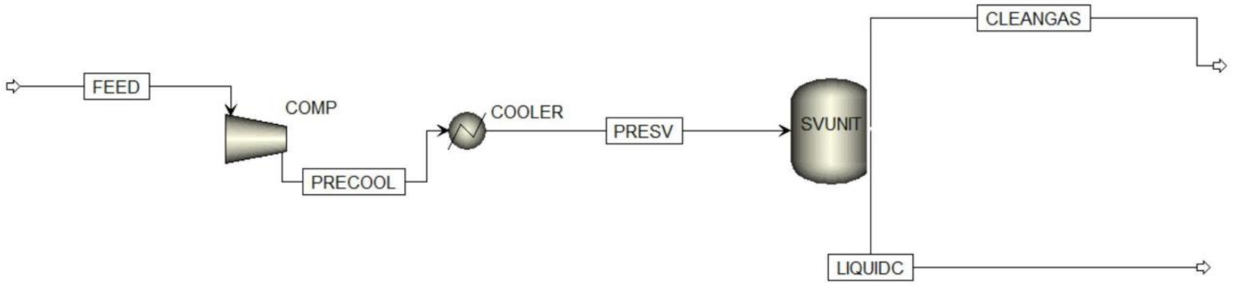
Desublimation offers the advantages of easier ability to retrofit existing power plant facilities, simplicity of design in that minimal other chemicals are needed, and the possibility of integrating NO_x and SO_2 removal. Additionally, desublimation produces pure CO_2 at temperatures close to liquefaction, offering less energy demand to liquefy and transport the product CO_2 via trucks or pipeline - an advantage for power plant facilities far from carbon capture and storage (CCS) locations.

Figure 1. Solid-vapor separation unit of CO_2 from flue gas using desublimation (Ababneh et al., 2022, p. 7).



Previous papers have explored the feasibility of using desublimation technology on feed streams containing N_2, O_2, and CO_2. Shown in Figure 1, a solid-vapor separation unit is used to separate the solid CO_2 from the flue gas through desublimation. The decrease in pressure as the stream enters the SV unit results in a decrease in temperature, allowing the CO_2 to solidify from the vapor state. The solid CO_2 is then heated on a melting tray to produce liquid CO_2 that flows out of the bottom of the unit. This study plans to expand on the process modeled in Ababneh, AlNouss, and Al-Muhtaseb's paper in Figure 2 to include NO_x, SO_2, and H_2O removal in the process.

Figure 2. Process flow diagram of solid-vapor PCC process from feed stream of N_2, O_2, and CO_2 (Ababneh et al., 2022, p. 14).



The aim of this project is to design a PCC plant to capture CO_2 in compliance with DOE's specifications using CO_2 desublimation technology. The design should include NO_x and SO_2 removal. The feed stream will be a typical power plant flue gas stream. The product CO_2 stream should meet requirements for CCS.

Considerations

The capital costs of the equipment and operating costs of the facility should be estimated and compared to existing PCC technologies. Reasonable assumptions about site classifications can be made, including local site conditions and available utilities. These should be well-documented to provide information on the type of facility this PCC technology will be best suited for. The techno-economic analysis should consider DOE funding for the project.

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5. Polyhydroxyalkanoate (PHA) Production From Plastic Waste (Recommended by Rosangelica Mancini-Lander and Richa Patel, Penn)

Background

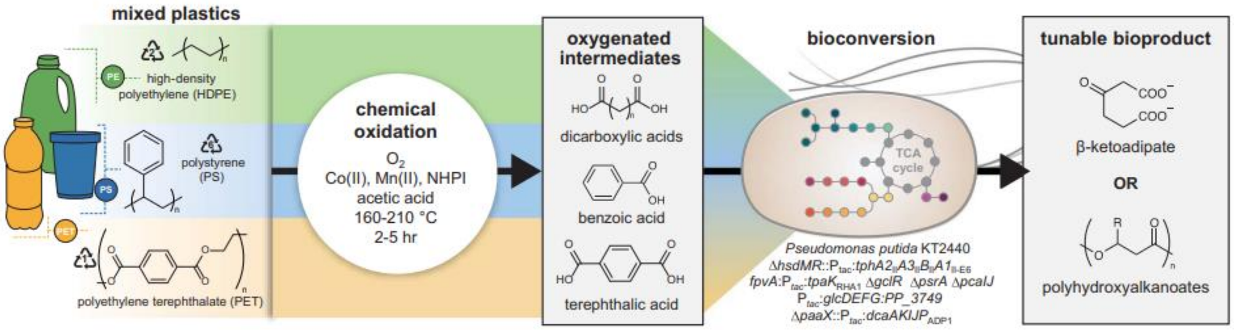
Plastic pollution is becoming an increasingly important issue facing climate scientists in recent decades. In 2022, scientists found 2.4 to 10.8 billion pounds of microplastic in the top foot of ocean water alone (Bergmann et al., 2022). Although small, these microplastics pose potential physical and toxicological risks to organisms since they can enter cells or tissue (Lim, 2021).

One of the most intriguing solutions to the imminent microplastics problem is biodegradable plastics. These plastics can readily break down into non-harmful materials significantly faster than typical oil-based plastics. Polyhydroxyalkanoate (PHA) is one of the most promising bioplastic options. PHA, unlike other biodegradable options such as polylactic acid (PLA), is 100% biodegradable in marine environments. It is completely non-toxic and degrades into materials safe for aquatic life (Creative Mechanisms Staff, 2017). PLA, however, is only biodegradable under very specific conditions which means it does not effectively address the issue of microplastics polluting the ocean (Miyauchi & Tsuji, 2018).

PHA has a wide range of potential applications from pharmaceuticals to food packaging and textiles (Chen et al., 2011). Additionally, compared to other bioplastics, PHA has a higher thermal resistance and various other positive mechanical properties that make it more favorable as a replacement for traditional oil-based plastics (Rajaram et al., 2022). Consequently, the market for PHA has shown significant growth in the past few years. In 2022, the market for PHA was $81M in 2022 and is expected to rise to at least $167M by 2027; with a CAGR of 15.3%, this is promising market growth that could be accelerated by the emergence of innovative, economically viable PHA production processes (Markets and Markets Staff, 2022). However, although this is a rapidly growing industry, the current methods of synthesizing PHA utilize materials such as sugar or methane gas (Markets and Markets, 2022). These are not necessarily sustainable and, in many cases, are very difficult to scale due to the high cost of starting materials; current PHA manufacturers report that ~50% of production costs are due to the high cost of starting materials (Surendran et al., 2020).

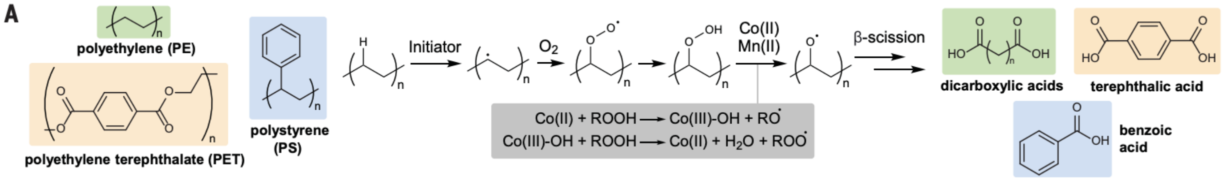
Project Proposal – Consumer Waste to PHA Conversion Process

In 2022, engineers at Oregon State in partnership with the National Renewable Energy Laboratory (NREL) published a paper in Science demonstrating a novel chemical process which converts consumer waste plastic (i.e. high density polyethylene (HDPE), polystyrene (PS), and polyethylene terephthalate (PET)) into PHA via catalyzed autoxidation and then fermentation by genetically modified bacteria, Pseudomonas putida (Sullivan et al., 2022). Researchers found that the yield of PHA produced from mixed consumer waste plastic was actually equivalent to, if not greater than the yields using commercially purchased organic acids, thus demonstrating the highly efficient nature of using waste plastic as a starting material (Sullivan et al., 2022). With this project, we aim to suggest a method through which to successfully scale up this chemical reaction from its current laboratory scale. The overall reaction is pictured in the figure below.



(Sullivan et. al, 2022)

The initial portion of the reaction is a chemical oxidation to convert the mixed plastic waste into PS-, HDPE- and PET-derived oxygenated intermediates. The mechanism of this reaction is depicted below. These organic acid intermediates are advantageous for the biological process to follow, due to their known metabolic pathways.



(Sullivan et. al, 2022)

The second half of this reaction is a bioconversion reaction using engineered Pseudomonas putida to biologically funnel the oxygenated intermediates into PHA.

The paper demonstrates the effectiveness of this reaction at a laboratory scale, but it is unclear whether the authors have tried to scale this process since the paper was published. However, the supplementary files for the paper contain a significant amount of data about the reaction kinetics and temperature dependence. They indicate that both as temperature and time of the reaction increase, the amount of moles of carbon product that result from initial deconstruction of the feed also increase, up until a certain point where they then stagnate. For temperature, this is at 170°C, and for time, at 3.5 hours .

Overall, this chemical process is extremely innovative due to its pairing of chemical and biological catalysis to create biodegradable plastics from plastic waste. The main reason that plastic is sent to landfills rather than being recycled is due to the costly and time-consuming separation process required in order to recycle each plastic – traditional recycling methods often involve melting down pure, individual plastic varieties (Sullivan – NPR, 2022). Thus, using a feed stream of mixed recycled consumer material has the potential to reduce the cost of starting materials as it is readily available from waste collection centers, and make PHA a more economically viable replacement to typical consumer plastics.

This process of PHA production has a consistent yield between a mixed waste and pure waste feed stream, which is a key differentiating factor between this process and more classical recycling methods, as mentioned above. Therefore, the scale-up of this process has the potential for a twofold environmental benefit: it could increase availability of PHA for use across various industries while also reducing existing plastic waste using a more efficient recycling method.

Problem Statement

Design a plant that will take this process to production scale. The feed stream will be mixed plastic waste made up of equal parts PET, HDPE, and PS. The goal would be to convert 11,000 tons of plastic waste per annum into PHA plastic using the dual reaction depicted above. This number is based on the collection of waste in local Philadelphia materials separation facilities, such as Waste Management and the Recommunity Recovery Center, which is around 1,200 tons per week (Rinde, 2022), and the percentage that plastics suitable for this reaction composes of this waste, 18.7% (Plastics: Material-Specific Data | US EPA, 2023). This leads to about 62,400 tons of waste being collected per year, with 11,000 tons being the plastic feed. You may assume the waste is clean and estimate the price accordingly.

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6. Hydrogen Production from Efficient Two-Step Water Splitting (Recommended by Rohan Bagchi and Andreas Ghosh, Penn)

Background

Electrolytic hydrogen production is a promising field, but is currently limited, mainly due to its low efficiency. Traditionally, water electrolysis involves coupled half reactions:

$2H^{+}\ (aq) + 2e^{-} \rightarrow H_2\ (g)$

Eq. 1a: Reduction half-reaction

$2H_2O\ (l) \rightarrow O_2\ (g) + 4H^{+}\ (aq) + 4e^{-}$

Eq. 1b: Oxidation half-reaction

These oxidation and reduction reactions at the anode and cathode, respectively, occur at the same time in the same cell. This causes issues such as inability to separate products and limited possibilities for materials used. Another major issue is the possibility of explosions from mixing the two components.

A possible solution to this problem involves a two-step process. First, the anode is oxidized, and water is reduced. The second step reduces the anode by oxidizing water. This two-step, decoupling process has shown to yield hydrogen at low voltages (1.44-1.60 V) with higher efficiencies [1].

Problem Statement

The Electrochemical, Thermally Activated Chemical (E-TAC) Process is a promising alternative method for water splitting.

Benefits:

- Safer
    - Hydrogen and oxygen won’t mix, preventing an explosion
- More economically viable
    - Membrane not needed (membranes are expensive)
    - Compressors may not be needed, since the process operates at high pressures (pumping liquid water feed to approx 45 bar) [2]
    - Reduced capital costs and operating costs
    - Fewer constraints on material selection
- More efficient
    - Oxygen generated thermally (close to zero power loss) as opposed to electrically (approx 25% power loss) [2]
- Can be scaled up at high pressures
- Mitigates crossover so lower current densities can be used. As a result, intermittent power sources like solar and wind energy do not significantly hamper the process.
- More degrees of freedom
    - Other process parameters, not only the electrolyzers, can be optimized (see Fig. 3)

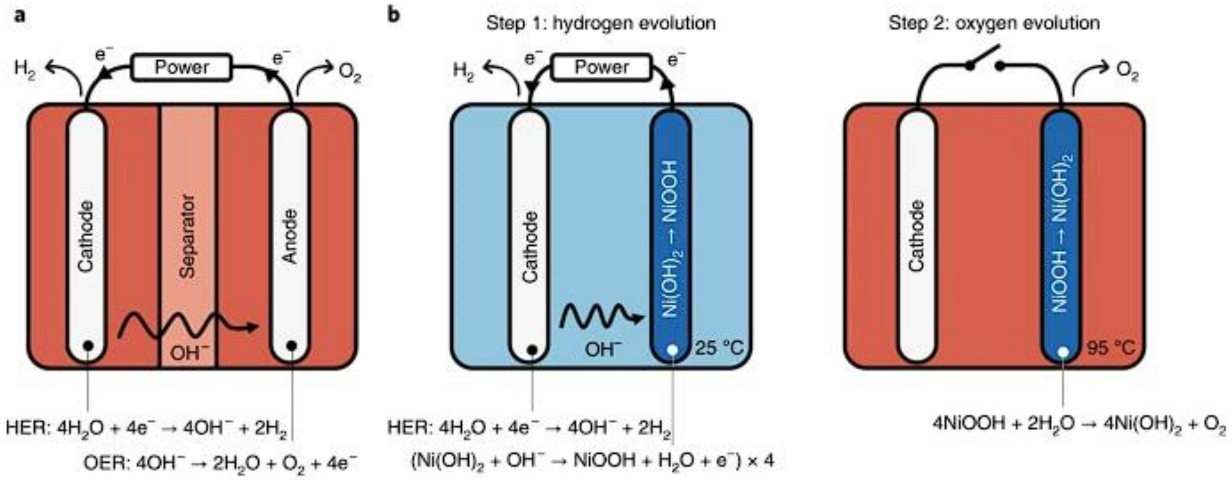

Fig. 1. a. Alkaline water electrolysis vs. b. Electrochemical, Thermally Activated Chemical (E-TAC) Splitting Process [1]. Note how in (b) the electrolysis process is two steps and a separator is not required.

Ref. [1] states that this E-TAC process is amenable to scaling up, but such a process has not been designed yet for large-scale use in industry. Your task is to design an industrial process that converts 250,000 gallons of water into hydrogen and oxygen per day. Your process should be some variation of current electrolysis processes, with a power source, a voltage transformer, an electrolysis stack, and a form of gas storage for the produced hydrogen and oxygen gas, like in Fig. 2 [3]. Note that in your process a separation of hydrogen from oxygen will not be needed. You should perform an economic analysis to estimate the profit from the plant after factoring in the cost of electricity required for operation.

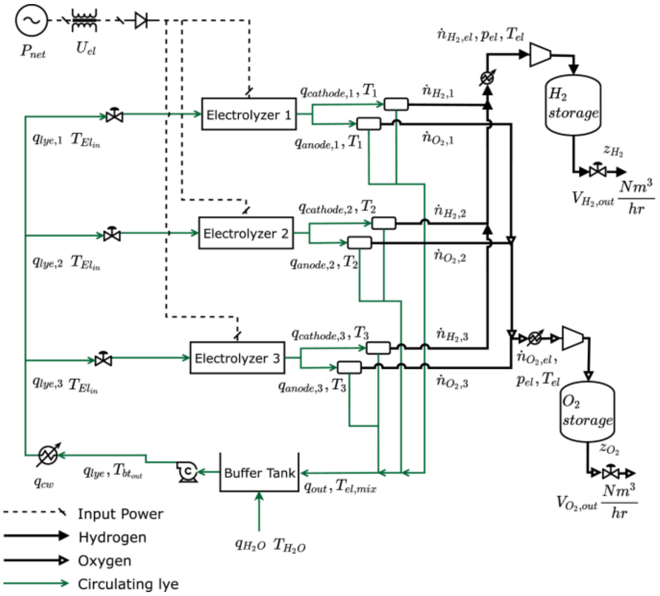

Fig. 2. A typical water electrolysis plant that takes in electrical power, converts the voltage to the required voltage for electrolysis, feeds the water to the stacks, and then separates and stores the hydrogen and oxygen products.

One potential design for this process was laid out in Ref. [1]. This "swing" process has three cells with three electrolytes: a cold electrolyte for the lower temperature steps, a hot electrolyte for the higher temperature steps, and an intermediate temperature fluid to move products into storage tanks. Each cell will use all three fluids in the process (see Fig. 3). Other operation modes, such as swap/swing and continuous, are possible for decoupled water splitting, but are still in research and development [1].

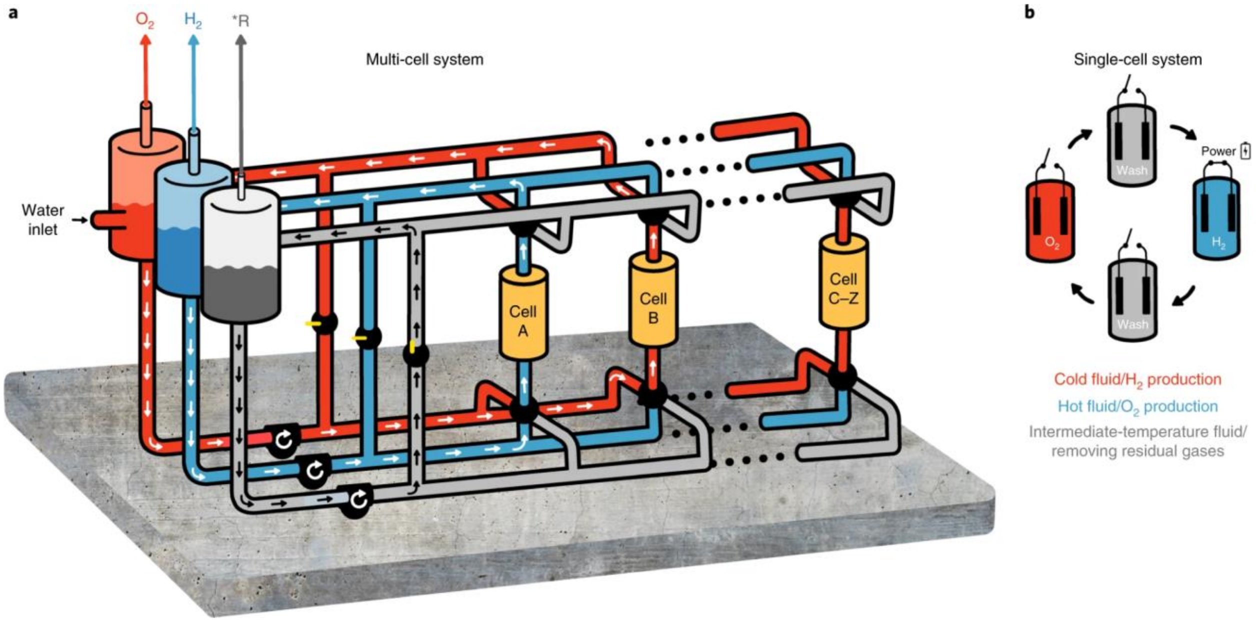

Fig. 3. Potential industrial design proposed by Ref. [1]. In this process (schematic in a), a high temperature fluid (red), a low temperature fluid (blue), and an intermediate temperature fluid (gray) flow through each cell at different stages in the process in a “swing” configuration. The desired products flow into the tanks on the left for further storage. Part b of the figure shows the E-TAC cycle for an individual cell.

The electrolyzers involved in this process will have several components that need to be carefully chosen and designed. Most industrial electrolyzers have the following parts:

- Bus bars
- Thermocouples
- Gas flow fields (to move product gasses through the cell)
    - Given the industrial design above, liquid flow should be considered instead
- Clamps/seals (to hold cell in place)
- Cathode/anode components (perhaps in layers)

You should have a working design and price estimates for all parts of these cells [4].

Assumptions

- Do *not* assume a constant operating voltage for this process. It may be a good idea to design a feedback loop that continually adjusts the voltage based on operating conditions
- You can take any relevant chemical data from the NIST WebBook
- Your nickel-based electrode can be the same as in Ref. [1], $Ni_{0.9}Co_{0.1}(OH)_2$.

Considerations

- Determine where your electrical energy will be sourced from. If it is from a renewable source, make sure that it is economically viable.

- Once you determine your source of energy, U.S. tax incentives (e.g. from Inflation Reduction Act sec. 45V) may apply [5]. These can have a significant impact on plant profitability.
- You may site the plant anywhere in the U.S. Construction costs, labor costs, cost and availability of renewably-sourced electricity, other operating costs, demand and transportation for the products, and state and local incentives will vary across different states and regions, so pay close attention to the above and any other relevant factors that may impact your location decision.
- You may need extra water for other parts of the process (e.g. heat exchangers). Make sure to factor this into your total water consumption.
- Investors will want to see at least a 15% IRR (internal rate of return) on this design. If that is not possible, propose possible design changes or process improvements or government incentives to make the process profitable.

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7. Food Production Without Photosynthesis

(Recommended by Jeffrey D. Cohen, Janssen R&D, Division of Johnson & Johnson)

Introduction

The objective of this project is to design and evaluate the feasibility of a process using large quantities of conventionally-produced chemicals e.g., methanol, methane, and ammonia. If the process has techno-economic merit it may serve as future motivation to generate these feed chemicals from renewable sources; however, renewable sources of the feed chemicals are out-of-scope in this project.

Background

The possibility of global food shortage due to demand and climate change-induced crop failures may be on the horizon. Food production without photosynthesis may become necessary [1].

Food is a composite of carbohydrates, protein, fats, and micronutrients. These composites can only be made by plants and living organisms. Humans cannot synthesize these composites directly from inorganic precursors that occur in the environment.

Three chemical elements make up the bulk of food: carbon, nitrogen, and sulfur, all of which are inaccessible to us in their inorganic forms: carbon dioxide and molecular nitrogen in the atmosphere as well as dissolved sulfate ions in soils and seawater. Other plants and organisms must first assimilate, i.e., fix these elements into their biomass as carbohydrates, proteins, and fats before we then can acquire those macronutrients by eating these.

Up until the early 20th century, all nitrogen, ultimately protein, that we derived from food was originally fixed by specialized bacteria in soils and the oceans. Even with the advent of industrial nitrogen fixation humans still rely on plants, fungi, and various microorganisms to convert inorganic nitrogen compounds into protein. Sulfur, which humans acquire as protein, can be assimilated in its inorganic forms by most organisms except for animals. [1]

We do not suffer a carbon shortage for food production. What is limiting are edible forms of carbon.

What limits global food production capacity is the rate at which CO2 is converted into biomass. In addition, most biomass is in the form of cellulose, not directly accessible as we cannot digest it. Livestock are biocatalysts for the conversion of indigestible plant materials into meat and dairy products.

The theoretical upper limit for current global food production is determined by the photosynthetic capacity of the planet. The total amount of CO2 converted into biomass on land and sea is known as net primary production (NPP), which has been estimated at 105 billion tons of carbon per year. However, these 105 billion tons are not fully accessible to us for food production. At present, the proportion of NPP already appropriated by humanity for food, fuel and fiber has been estimated at 25%. Due to the biophysical constraints of agriculture, i.e., the need for arable land, sunlight, fresh water, and favorable climate conditions, this number may be difficult to increase much further. [1]

Photosynthesis has an absolute dependence on light energy. Food is unavailable from sunlit farmed acreage growing annual crops between the time periods of harvesting.

A goal may be to allow for continuous carbon, nitrogen, and sulfur fixation by employing a way to convert these to edible biomass independent of photosynthesis by breaking the NPP barrier. [1]

Edible microbes produced chemosynthetically may decrease full dependence on photosynthesis.

There are several possible options for how edible microbial biomass could be produced from organic compounds. Methanol is the simplest alcohol and can be produced by monooxygenation of methane. Many microorganisms can grow using methanol or methane as the sole source of metabolic carbon. These microbial species are methanotrophs [2,3].

During the 1970s and 80s, the British company Imperial Chemical Industries developed a high-protein animal feed called Pruteen, which was derived from the edible methanol-assimilating bacterium Methylophilus methylotrophus [4]. Ultimately Pruteen production was discontinued due to rising methanol prices and competition from cheaper soy-based feeds. Nevertheless, the Pruteen process demonstrated that it was possible to produce edible microbial biomass in significant amounts, 50,000-60,000 tons per year, from a single 1,500 m^3 bioreactor. Recent estimates indicate that if the entire US soy production capacity, about 120 million tons per year, was to be replaced with methanol factories and Pruteen-style bioreactors, it would occupy roughly one thousandth of the same land area. Note: this estimate does not include energy sources to power the methane oxidation, conversion process. The land-sparing potential of such a process would depend heavily on the power density of the chosen energy source.

To produce 50,000 tons of soybeans per year, requires about 37,500 acres of arable land. To replace the entire current soybean production capacity in the US, i.e., 90 million acres would require a Pruteen-like process composed of 2,400 bioreactors [1].

In the past Statoil, Inc. and presently Calysta [5,6] committed to SCP production using methane. These corporations see merit in using methane due to wide availability despite the additional challenges associated with using methane versus methanol, e.g., low solubility in aqueous media, higher heat of reaction, higher oxygen requirement, safety issues, etc. Calysta has plans for constructing manufacturing facilities in the U.S. and partnerships in China [7].

Project Objective

The objective of this project is to perform a techno-economic analysis of two (2) single cell protein (SCP) processes, comparing the use of two (2) carbon sources: methanol versus methane. The techno-economic analysis shall quantify capital investment, operating cost, and estimate profitability. In both cases the biocatalyst, growth media, separation, drying, and packaging unit operations may be essentially the same. What differs, in both cases, is the bioreactor and the associated details affecting rates of mass, heat, and momentum transfer. Figures 1 and 2 below give examples of bioreactor types suitable for methanol and methane carbon source respectively. Additional details to consider in the process comparison are differences in methanol versus methane:

- Solubility in aqueous media in which the cell suspension accumulates
- Enthalpy of reaction
- Meeting Oxygen Transfer Rates to meet biological Oxygen Uptake Rates
- Mitigating process hazards

As a benchmark, SCP price may be compared with, for example, price for soy protein.

Assumptions:

- Case 1 and Case 2: Methanol [8] and methane [9] used as carbon sources respectively
- Both cases: Anhydrous ammonia [10] used as nitrogen source
- Remaining growth media components: cell line dependent, to be determined by cell line selected

- Biocatalyst doubling time: cell line dependent
- Bioreactor production mode: batch or continuous
- Final product form: dry SCP particulate
- Annual production rate per production facility: 50,000 tons SCP bone dry basis
- Production uptime: 50 weeks/year
- Bioreaction is aerobic, exothermic, operated sterilely
- Final product packaged dry in supersacks
- Final product for human or animal consumption, affects selling price

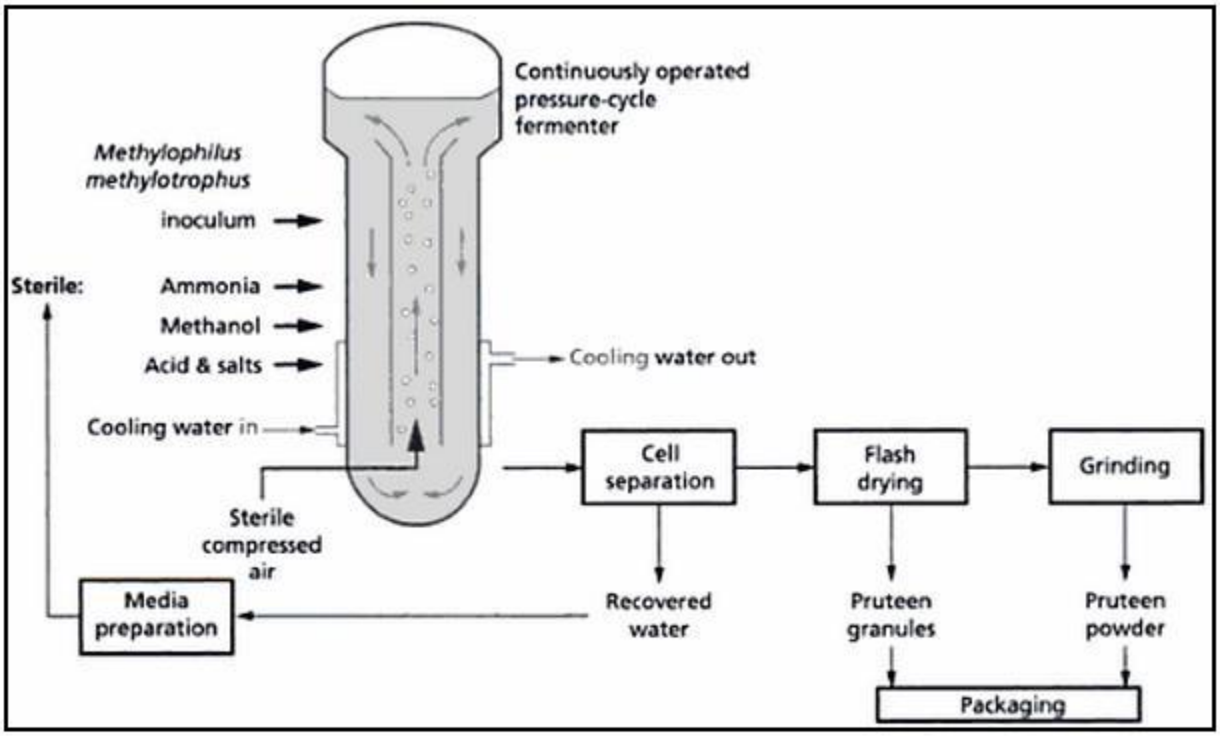

Figure 1. ICI Pruteen Air lift bioreactor, Pressure Cycle Fermenter. Example of methanol-based process [4].

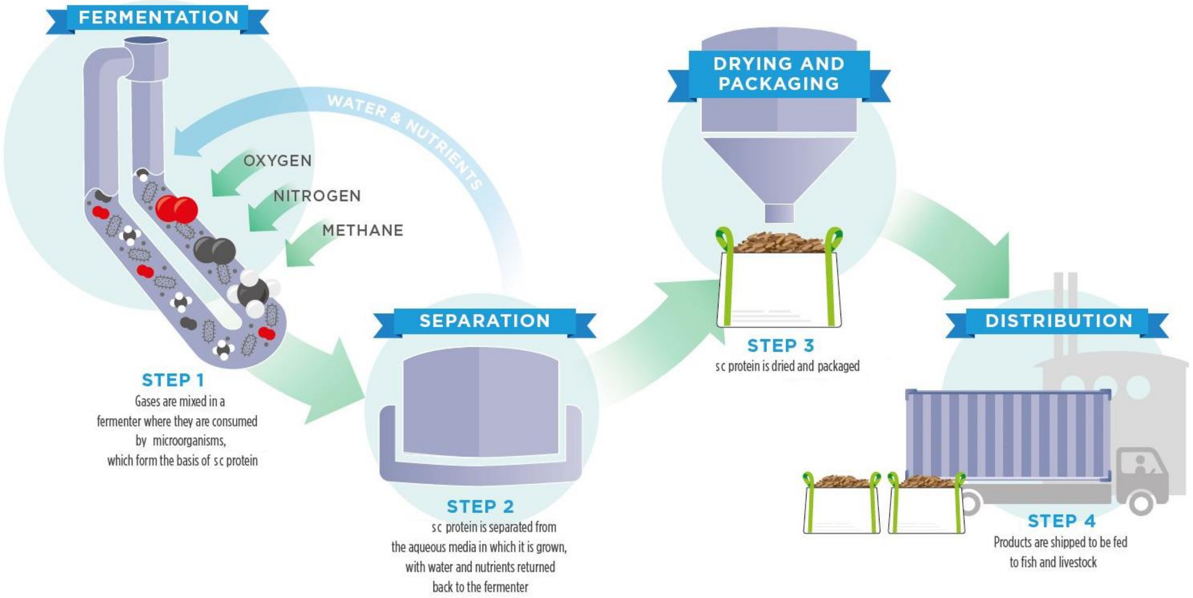

Figure 2. Calysta, Loop Bioreactor to produce Feedkind®. Example of methane-based process [5].

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8. Neopentyl Glycol Production
(Recommended by Stephen M. Tieri, DuPont)

Introduction

Neopentyl Glycol (NPG) is a key component for the production of polyester resins for industrial coatings, in addition to lubricants, pharmaceuticals, and plasticizers. NPG provides the resins with overall toughness, stain & detergent resistance, and strong outdoor weathering performance. Resin powder coatings (produced with NPG) are viewed as environmentally friendly, as they typically have significantly lower emissions (up to 50% lower), compared to traditional liquid coatings.

Background

Commercially, NPG is produced by first reacting isobutyraldehyde with formaldehyde in the presence of a ternary amine, producing hydroxy pivaldehyde (HPA). After stripping, the HPA is hydrogenated to NPG. Commercially, NPG is supplied in three typical forms: as flakes (solid), molten (100%), and as a 90% liquid solution. Flakes are supplied in bags (1 MT supersacks), while the molten and 90% liquid solution are sold in bulk tank trucks. By using biobased raw materials and/or renewable energy, the potential exists to produce an NPG product with a net zero carbon footprint.

Your company is a major global NPG producer, and is currently forecasting a continued increase in demand in the resins market. To support the growing demand in Asia and powder coating market/applications, and strengthen their position as a leading NPG supplier, the company has decided to expand NPG production capacity in the region, with a new facility in Singapore.

Problem Statement

Your team has been assembled to design the new world scale NPG facility, employing the most current, efficient, and sustainable technologies. However, the choice between traditional NPG, “Low Carbon Footprint” NPG, and “Net Zero” carbon footprint NPG has not yet been made. While the company’s preliminary economic forecasts indicate significant economic potential from this additional NPG capacity, the results and recommendations from your team’s economic analysis of the final design will be used for project approval. Additionally, the business leaders will rely on your team’s work to make the choice between traditional, “Low Carbon Footprint” NPG, and “Net Zero” carbon footprint products.

The project’s business objective is to design a new world facility to produce 80,000 MT/yr of Neopentyl Glycol (dry basis). The NPG must meet or exceed current commercial requirements for resin grade purity and quality (ex. 99.8 wt %, moisture, and low APHA color) to be acceptable to the market and customers. The facility is expected to have capability to deliver product in all three typical forms. Current market pricing is to be expected for NPG product(s), raw materials, and utilities.

In addition to detailed process equipment and unit operation designs, the completed project is expected to include estimates of facility investment, expected operating costs, revenue, business profits, and overall project financial performance. Your team is responsible for identifying and minimizing the required investment, operating costs, optimal product mix, and identifying any critical economic sensitivities to raw materials, product mix, utility consumption, equipment pricing, or product/co-product pricing. The design and investment estimates should include appropriate equipment and systems for raw materials feed and product storage capacity. The proposed new facility will be in located in Singapore.

The plant design should be as environmentally friendly as possible, and as necessary as required by local, state, and federal emissions legislation. It is expected that the facility will include emission control equipment as a part of the identified process design and operation. Recover and recycle process materials to the maximum economic extent reasonable. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. As the process technology evaluation, integration, and design team, you will be there for the start-up and will have to live with whatever design decisions you have made.

You will need additional data beyond what is provided above and listed in the references below. Cite any literature data used. If and when required, make reasonable assumptions, state them, and identify to what extent your design or economics are sensitive to the assumptions you have made.

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9. Tritium Removal from CANDU Reactors
(Recommended by Ella Siefken and Phuong Ngo, Penn and Adam Brostow, Chart)

Background

CANDU (**Can**adian **d**euterium **u**ranium) reactors use heavy water (deuterium oxide) as a moderator and coolant and natural uranium as a fuel to generate electricity.

Tritium, a radioactive isotope of hydrogen, is a byproduct from CANDU reactors generated through the interaction of fission neutrons with heavy water. A typical CANDU reactor produces about 130 g tritium per year. The generated tritium can be extracted from the heavy water moderator and coolant with Tritium Removal Facilities (TRFs) that take CANDU moderator as primary feed [1].

Tritium is a vital component in the ongoing research for nuclear fusion reactions, which has recently seen significant developments at the National Ignition Facility, where researchers generated a breakthrough net positive nuclear fusion reaction [2]. Extracted tritium is also useful in various applications, including radioluminescent devices, biomolecular tracing, and weapons development. The extraction of tritium also reduces the radiation safety implications of releases of moderator water and prevents reactor inefficiencies that can accompany diminished deuterium concentrations (<99.8%) in moderator fluid.

Problem Statement

Students will analyze the Bruce Nuclear Generating Station located in Ontario, Canada and design a joint tritium removal facility that would operate concurrently with the nuclear power station. The resulting process will take 200 kg/h of tritiated heavy water feed and produce tritium with a greater than 99% isotopic purity that can be stored for further research and industrial applications.

Basis of design

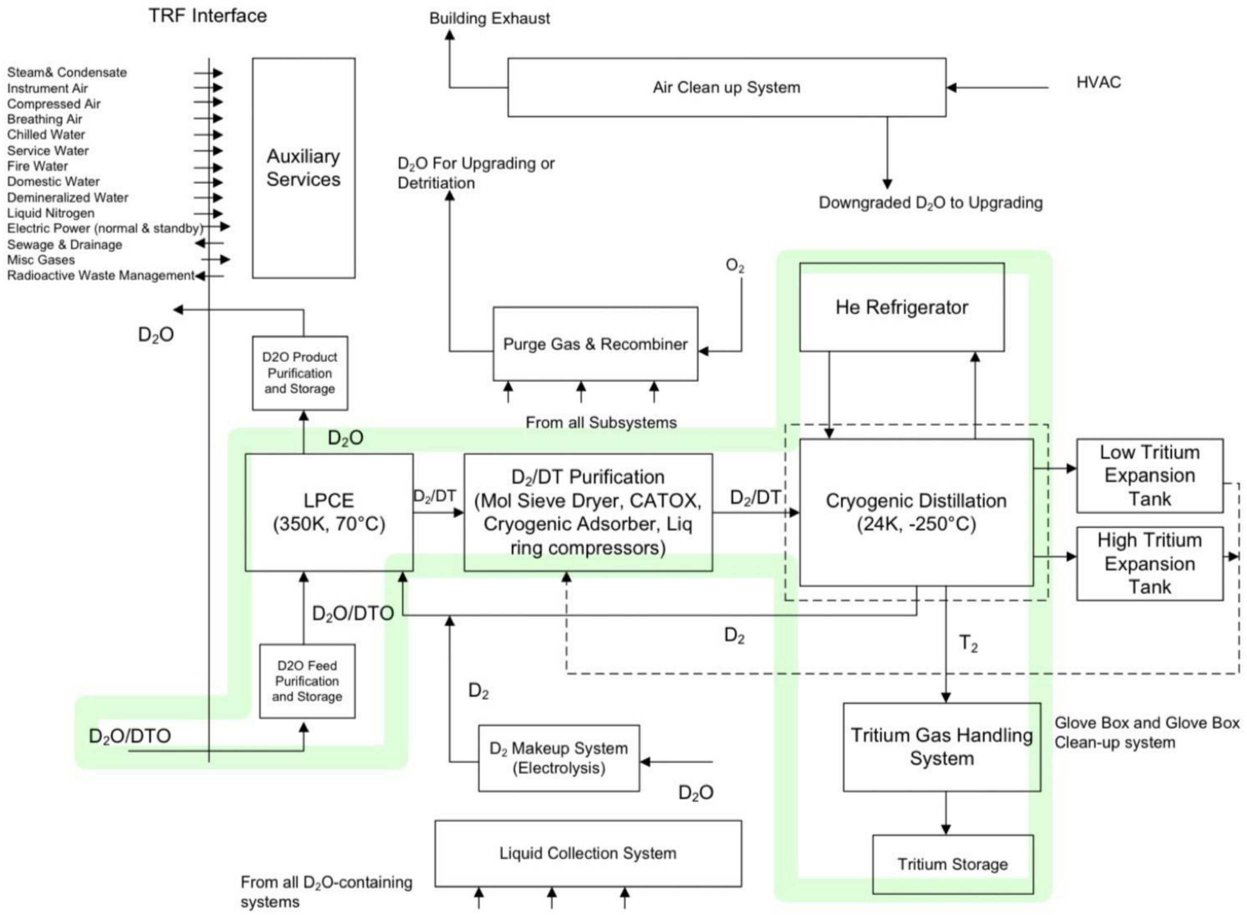
At plant maturity (~40 years), the tritium concentration in moderator may be as high as 150×10^{10} Bq/kg. At Bruce generating station, where reactors have been in operation for between 36 and 43 years old, moderator tritium concentration can be approximated by this value.

The Wolsong tritium removal facility (WTRF) consists of four CANDU reactors, and was designed to process 100 kg/hr of tritiated heavy water feed to produce 99% pure T_2 [3]. Similarly, the TRF at the Bruce Generating Station, with eight CANDU reactors, may be designed to process approximately 200 kg/hr of tritiated heavy water to remove T_2 of the same purity.

The TRF designed by the group will resemble the process depicted in Figure 1 [4]. The process is designed to include the 4 main process units that appear in existing facilities (WTRF, DTRF, CTRF): catalytic exchanger, purification unit, Cryogenic Distillation (CD) stack, and metal hydride storage. The front end process of the TRF will be a liquid phase catalytic exchange (LPCE) maintained at a temperature of about 350K, as seen in the process depicted in Figure 1.

The front end of the TRF can be a LPCE unit, where tritium is extracted from heavy water to the deuterium gas phase through catalytic reaction. The WTRF LPCE consists of two packed-bed columns, which have separate catalysts and packing for two step exchanges between tritium and deuterium. Some feed and product specifications for the WTRF LPCE system can be found in Reference [5].

Figure 1.



The cryogenic distillation (CD) system contains the catalytic conversion equipment that would produce T_2 from the purified LPCE output (D_2-DT mixture). The DT chemical equilibria demonstrated in Reaction 1 (below) occurs in the CD system, and the calculated equilibrium constants for temperatures between 19.7K and 1000K can be found in reference [6].

$$D_2 + T_2 \rightleftharpoons 2\ DT \qquad \textit{Reaction 1}$$

D_2-DT separation factors and other relevant parameters (including UNIQUAC model parameters) are also presented at various temperatures in references [7] and [8]. Due to the lack of azeotropic points on the e-H_2/e-D_2 liquid vapor curve, it can be assumed that D_2-DT-T_2 will form a single solution. All species should be in the liquid phase, and D-T behavior can be estimated based on the triple line phase diagram of H-D behavior [6]. Table 1 contains detailed information about inlet and intermediate streams.

Table 1: Stream Compositions

	Flow rate, kg/h	Pressure, kPa	Temp, K	x_{HDO}	x_{HTO}	x_{DT}
D_2O/DTO Inlet	200	145[a]	350	2.0×10^{-3} [b]	2.7×10^{-5} [b]	–
D_2O/DHO outlet (bottoms)					5.4×10^{-7} [c]	
D_2/DT Purification Inlet	50-400[d]	120-145[e]	350	–	–	1.08×10^{-4} to 1.35×10^{-5} [g]
CD Inlet	0.0125[f]	133[f]	23-26[f]	–	–	**

a) Reference [10]
b) Mole fractions taken from reference [10] and scaled based on a mature plant moderator concentration of 40 Ci/kg.
c) Based on a target Detritiation Factor of 50.
d) See reference [10]. Flow ratio of feed hydrogen to water varies based on column specifications.
e) Reference [5]
f) Reference [12]
g) Based on simple T balance, range based on D_2/DT outlet flow rate ** Find the CD inlet composition using D_2O/DHO outlet after analysis.

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10. Sustainable Aviation Fuel
(Recommended by Jacob Sheldon and Mitch Walker, Penn)

Introduction

The aviation industry accounts for roughly 2% of all global greenhouse gas emissions and is the fastest growing transportation mode in recent decades. They have pledged to reduce carbon emissions to net zero by 2050 thus highlighting the desperate need for abatement. A promising method explored by the industry is sustainable aviation fuels (SAFs). SAFs are biofuels produced from non-fossil based feedstocks such as food and plant waste. Every year, 119 billion pounds of food is wasted which could now be repurposed as alternative jet fuel. Part of what makes SAFs so attractive, apart from their ability to reduce carbon emissions, is how easily they are integrated into the current aviation infrastructure. These biofuels have the same chemical makeup as the initial jet fuel allowing for current planes to use them without any modifications.

Gevo is a company that is currently pursuing sustainable aviation fuels. They have agreements with airlines and other partners, however their technology has not yet been fully commercialized. They produce SAFs through a process they call Alcohol-to-Jet Synthetic Paraffinic Kerosene (ATJ-SPK). The process takes ethanol and isobutanol and refines them into SAFs through three steps: dehydration, oligomerization, and hydrogenation. The dehydration process removes the oxygen from the chemicals through water, leaving isobutylene. Oligomerization causes the compounds to combine forming C8 and C12 olefins which are then readily hydrogenated into hydrocarbon products.

Problem Statement

Your employer, a major airline, is considering partnering with Gevo to fulfill its ambitious carbon reduction targets. Your group has been assembled to design a process to make 100 million gallons of SAF using the Gevo technology to determine its economic viability before your CEO decides to meet with Gevo to discuss working together, or decides to invest in other competing technical options, or decides to retire and cash out their stock options. Your team must assemble the design based solely on public information and the several relevant patents assigned to Gevo. So as not to tip off your company's interest, there can be no contact with Gevo or others (except for industrial consultants and faculty at Penn).

Since the data available to you is far from complete, you are going to need to identify major uncertainties and make many assumptions to complete the design. To give your CEO the full picture, explicitly state your assumptions in the report so that they may understand the uncertainty in the design and economic projections for when they discuss a possible partnership with Gevo. Your economics should be tested to a reasonable range of your assumptions. If there are any assumptions that, if incorrect, would make the design infeasible or uneconomical it must clearly be understood and communicated before continuing with the project.

The plant can be located anywhere within the United States. You will want to consider the logistical costs of the feedstock ethanol as well as the SAF product, construction costs, labor costs, and energy costs amongst other things. Look into the possibility of discounted ethanol by being located near a few large ethanol plants. Be aware of some regulatory hoops you may have to jump through (Bureau of Alcohol, Tobacco, Firearms, and Explosives rules around denatured vs. undenatured ethanol).

As the company wants this venture with Gevo to be a profitable one, calculate the required green premium compared to conventional jet fuel in order to achieve a 15% IRR on the investment. Then, determine whether this is a feasible investment that you would recommend for the company and pitch your decision to the CEO.

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