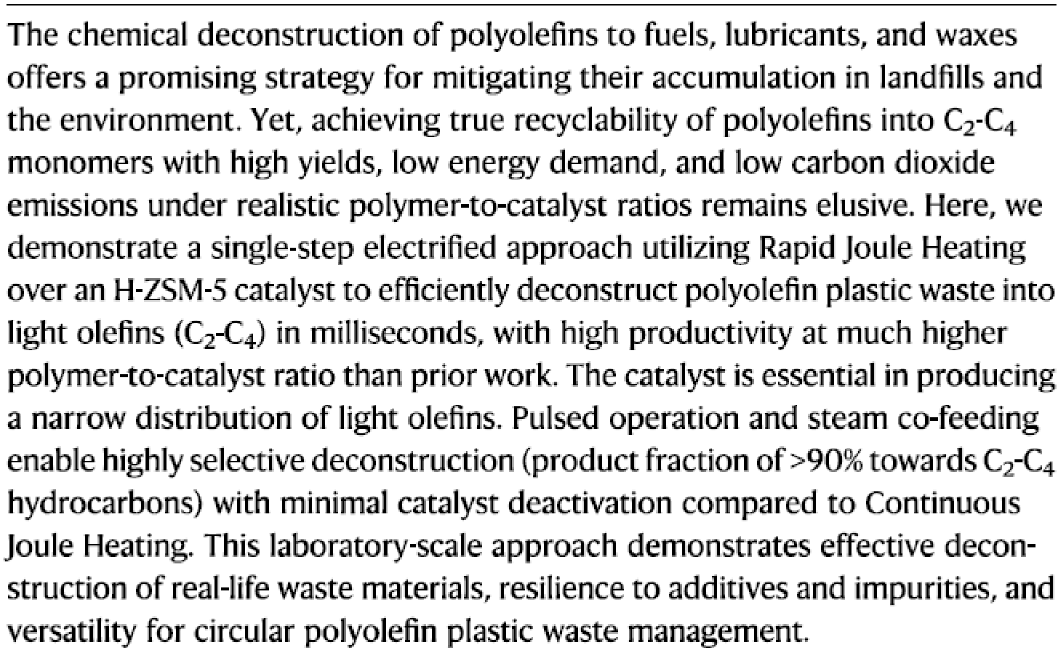
Suggested Design Projects – 2024-2025

1. Circular Polyolefin Plastic Waste
(Recommended by Leonard Fabiano, Adjunct Professor, Penn)

Background

Plastic waste is one of the most vexing problems facing society today. The amount of polymer waste in the oceans is well documented. Polyolefin wastes (polyethylene, polypropylene, etc., used in grocery bags and other packaging, for example) are one of the least recycled plastics for a variety of reasons. And what is recycled is often downcycled into lower value applications, requiring more virgin polymer to be manufactured.

A recent Nature Communications paper discusses a new process to convert polyolefin waste into monomers with high yield, low energy demand and thus low CO_2 footprint. The abstract, copied here, summarizes the work well.



> The chemical deconstruction of polyolefins to fuels, lubricants, and waxes offers a promising strategy for mitigating their accumulation in landfills and the environment. Yet, achieving true recyclability of polyolefins into C_2-C_4 monomers with high yields, low energy demand, and low carbon dioxide emissions under realistic polymer-to-catalyst ratios remains elusive. Here, we demonstrate a single-step electrified approach utilizing Rapid Joule Heating over an H-ZSM-5 catalyst to efficiently deconstruct polyolefin plastic waste into light olefins (C_2-C_4) in milliseconds, with high productivity at much higher polymer-to-catalyst ratio than prior work. The catalyst is essential in producing a narrow distribution of light olefins. Pulsed operation and steam co-feeding enable highly selective deconstruction (product fraction of >90% towards C_2-C_4 hydrocarbons) with minimal catalyst deactivation compared to Continuous Joule Heating. This laboratory-scale approach demonstrates effective deconstruction of real-life waste materials, resilience to additives and impurities, and versatility for circular polyolefin plastic waste management.

Problem Statement

All the work so far has been done at laboratory scale. Normally, scale-up to commercial scale directly from the lab is neither practical nor wise; companies usually go through several intermediate scale-ups. However, your company, a large polyolefin manufacturer, is willing to consider taking that risk due to the importance of the problem to society, to gain a competitive advantage, and to try to avoid regulatory interventions that would disrupt your business.

A waste management firm handling a significant fraction of the waste in Philadelphia has approached your company, offering to sell 10MM kg/yr of clean, granulated polyolefin suitable for depolymerization.

They will run the supply chain and deliver to your site trucks of free-flowing polyolefin waste for $50/mt, after considering their costs plus the revenue they receive from their waste disposal business.

Design a plant, using the process described in the reference, to depolymerize the polyolefin waste to make polymer grade olefins and estimate the profitability. You may include in your economics a selling price with a reasonable green premium for the olefins (although your product will likely be consumed by your company and not sold to a competitor). Test the sensitivity of your economics to both the $50/mt fee you pay and the green premium. Should your economics not indicate at least a 15% IRR, determine the feedstock purchase price you would need to negotiate with your supplier, or the green premium you would need to charge your (internal) customer, to achieve 15% IRR.

Because the research is early stage, you will need to make, document, and justify many assumptions in your report to management. Determine the strengths and weaknesses of the published data. And describe what future research must be done before this plant can be built.

The paper describes conditions that you can vary that lead to different ranges of C_1 to C_8 products. One of the first things you should do is decide on the product slate you want to design the plant for, possibly based on some economic calculation. Although you will likely not have sufficient time to design for multiple product slates, your final report to management should recommend an optimum product slate (most profitable or desirable for another reason) - even if that product slate is different than the slate you designed the plant for.

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. All products and coproducts must meet market specifications. Waste streams from purges or other streams should be identified with appropriate treatment and cost before release into the environment. Energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate.

Reference

E. Selvam et. al., Recycling Polyolefin Plastic Waste at Short Contact Time via Rapid Joule Heating, Nature Communications, 2024, https://doi.org/10.1038/s41467-024-50035-3

2. Utility and System Design for Green Ammonia
(Recommended by Gary Sawyer, Process Evaluations LLC)

Introduction

Green chemistry focuses on the use of renewable energy to power a process with low or no carbon footprint. Processes connected to a power grid use electricity from a mix of fossil fuels, nuclear, hydroelectric, solar, and wind generation. Small, modular processes – particularly those in remote locations – can be designed to include off-grid, renewable electricity generation. Ammonia, a key ingredient in fertilizers, is of particular industrial interest for green chemical synthesis.

Ammonia

Ammonia is made by reacting hydrogen and nitrogen according to:

$$N_2 + 3\,H_2 \Leftrightarrow 2\,NH_3$$

This is an endothermic, equilibrium-limited reaction known as the Haber process. Conversion is favored by high pressure and temperature (Torrente-Murciano, n.d.). Conventional large scale ammonia synthesis uses natural gas as a source of hydrogen, generating significant quantities of CO_2. Alternatively, hydrogen can be generated by water electrolysis.

In the conventional process, nitrogen is recovered from spent combustion air, after the CO_2 has been removed. Alternatively, an air separation plant can be employed for nitrogen generation.

Wind and Solar Utility Systems

Figure 1 below is a schematic of the components of a wind/solar utility system supplying a dedicated customer (or process in this case). Battery storage supplies the process when there is no sun or wind. Both wind and solar generators produce DC current, which must be inverted to AC current for most industrial applications.

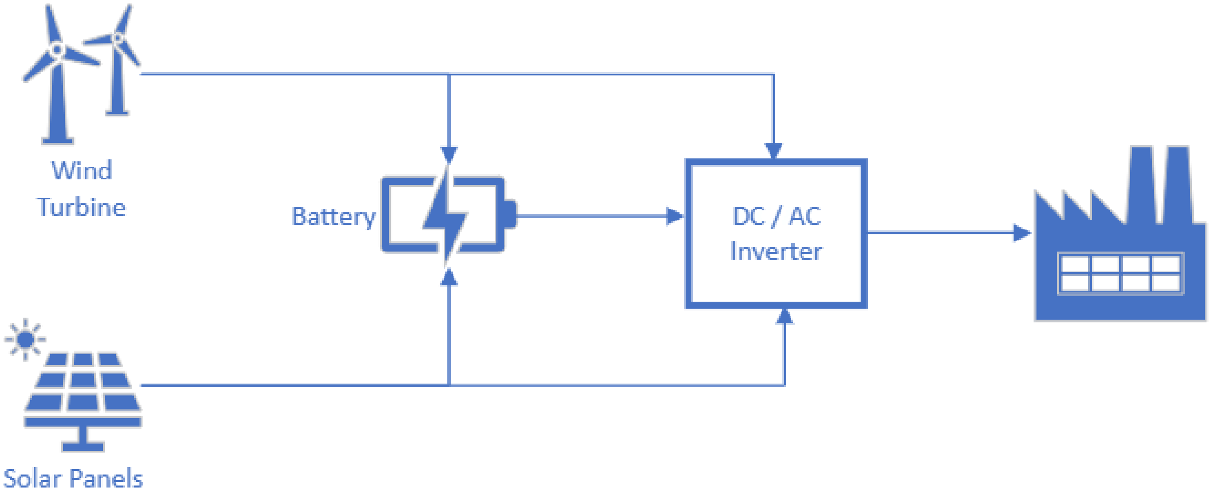


Figure 1 Components in an off-grid renewable energy generation project

The power generation from a wind turbine depends on the wind speed. A good source of data for power curves for various turbines is at wind-turbine-models.com . Note that wind turbines can be taller than the length of a football field, and wind speeds vary with elevation (Wind Profile Calculator, n.d.).

Photovoltaic (PV) solar panels will generate a DC power output of around 20% of the incoming solar radiation, based on standard test conditions with 1000 W/m^2 incoming solar radiation. Utility scale batteries return about 80% of the power that was used to charge them (Today in Energy, 2021). Inverters are about 96% efficient in converting DC to AC power (Vignesh Ramasamy).

The National Renewable Energy Laboratory (NREL) has several good publications for costs and efficiencies of the utility components mentioned above, including for wind turbines (Tyler Stehly), photovoltaics (Vignesh Ramasamy), and battery storage (Karmakar).

Weather Data

The National Oceanic and Atmospheric Administration (NOAA) has observation stations in the US that collect a wide range of weather data, including wind speeds and solar radiation on an hourly basis at over 200 stations in the U.S. (Index of weather stations, n.d.). There are other resources and maps of average conditions you may also find useful in locating your project.

Senior Design Project Description

Your project is to use historical weather data to size a wind and solar utility supply system to power a small-scale ammonia facility that includes the following process units:

- Hydrogen generation from water electrolysis. You don't need to design this system per se; you can assume it is supplied by a third party. You will need to know the capital cost and electricity requirements, as well as water quality specifications. Water treatment is also outside the scope of your project, but water usage may be a factor in your location decisions.

- Air separation plant to produce nitrogen. Again, you don't need to design the plant. You should understand which of two common separations, cryogenic or pressure swing adsorption, is better suited, in order to estimate capital costs and electricity requirements.

- Ammonia process. Here, you should design the process, selecting an operating pressure and temperature for the Haber reactor. You can assume that the reaction reaches equilibrium at the operating conditions you choose. Operating pressure will affect the ease of ammonia recovery. ASPEN simulations are useful in this part of the project.

A typical "green ammonia" plant size is around 450 metric tonnes per day (Stamicarbon press release, n.d.), but you may choose a different size.

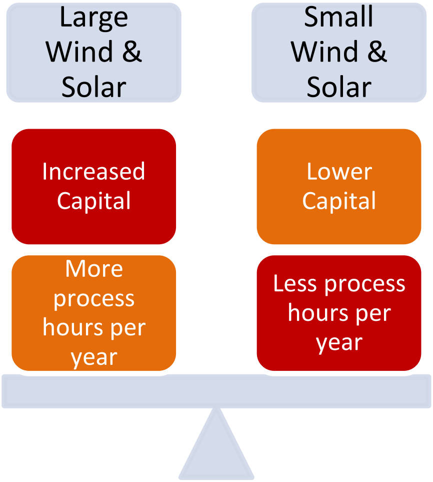
Bear in mind that the utility system will seem oversized for the process demands. That is, for example, a wind turbine capable of producing 3 MW at peak performance, may average something less than 1 MW over the course of a year. There will be a trade-off between the size of the utility system and the on-stream availability of the process. Ideally your utility system will not consume any fossil resources.

Your project should optimize the size of the utility system to supply the ammonia process, using a discounted cash flow analysis to determine the price of ammonia you should charge to get a 5% IRR on your investment. You should do sensitivity to other IRRs as well.

It is suggested that at least initially your group divide into three tasks:

- Select a location with good renewable energy resources and a source of water, preferably near potential agricultural customers. Develop a model for power generation, storage, and consumption using historical weather data near your location. Power generated minus power consumed = power accumulated (battery storage). Don't forget about battery efficiency.

- Collect information on electrolysis and nitrogen plant costs and electricity consumption.
- Develop a simulation model in ASPEN for ammonia synthesis. Study variables such as operating pressure and temperature on recycle flows, compressor sizing, and ammonia recovery.



Large Wind & Solar

Small Wind & Solar

Increased Capital

Lower Capital

More process hours per year

Less process hours per year

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3. Active Pharmaceutical Ingredient Production for Large Volumes (Recommended by Alex Marchut, Mineralys Therapeutics)

Background

With new large volume small molecules coming onto the market, the pharmaceutical industry is currently interested in large capacity production. Several factors will come into play when selecting what scales to build new manufacturing facilities at such as cost per kilo, demand and quality.

There are two small molecule Active Pharmaceutical Ingredients (APIs) known as Molecule A and Molecule B that are currently in development targeting obesity (and expected to have high demand in the US). Molecule A has a selling price of $5000 per kg and the cost of the penultimate intermediate is $3500 per kg. Molecule B has a selling price of $3000 per kg and the cost of the penultimate intermediate is $2500 per kg. Molecule A, based on its dosage and forecast is expected to be needed at 20 metric tons per year and Molecule B is expected to be needed at 40 metric tons per year. Unfortunately, Molecule A and Molecule B have quality risks and overall, between the different failure modes in each step, it is expected that Molecule A's synthesis will produce API that does not meet its specifications 2% of the time and Molecule B's synthesis will produce API that does not meet its specifications 0.5% of the time. For these APIs, when a batch does not meet the specifications there are no reprocessing or reworking procedures and the batch is a total loss.

Problem Statement

You will design two GMP manufacturing facilities to produce the two API's starting with the penultimate intermediate. In each case there is a reaction, followed by an extraction, a distillation, and a crystallization. The crystallization slurry is then filtered and dried. Technical data to design the facilities will be discussed in the initial meeting with the group.

One facility should be designed at 2000 L to 3000 L scale and the other facility should be designed at 12000 L to 15000 L scale for the reactors. The reactors should be designed so that all the steps from reaction to crystallization can be performed in two identical batch reactors. The isolation and drying should be done either in a filter dryer or a centrifuge and a conical dryer with the same type of isolation and drying done in both plants. Once you have designed the facilities you should examine the economics of running Molecule A in each facility and Molecule B in each facility. You can also perform sensitivity studies to see the impact of lowering the cost of the penultimate intermediates and lowering the batch failure rate. The selling price per kg of each API is fixed.

As you design the facilities, you should do your best to keep capital costs of the equipment and operating costs of the facilities to a minimum. You can build the plants anywhere in the world, but you should consider things like cost of labor and availability of dependable supplies of utilities such as electricity and water when you choose the location. The facilities should be designed so that the operators are safe from hazards like inhaling dust from the powders or fumes from the solvent or explosions from the powders or solvents and no waste is released to the environment. Note that if the smaller facility cannot handle the capacity, additional trains can be added, for example you can have two or three of each piece of equipment to make two or three production trains. You should assume that each facility is being retrofitted into an appropriate warehouse, i.e. that the walls and floors of the building have been built and you will focus on the production equipment.

4. Low/Net Zero Carbon Footprint Neopentyl Glycol Production
(Recommended by Stephen M. Tieri, DuPont)

Background

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 and 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.

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, while the molten and 90% liquid solution are supplied in bulk tank trucks. By using biobased raw materials and/or renewable energy, the potential exists to produce a NPG product with a net zero carbon footprint.

Problem Statement

Your company is a major global NPG producer, and 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.

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”, and “Net Zero” carbon footprint products.

The business team currently expects that traditional petrochemical feed materials will produce traditional NPG; using renewable feedstocks OR renewable energy will deliver “renewable” or “low carbon footprint” NPG, and that BOTH bio-based feedstocks and renewable energy are necessary to produce “Net Zero Carbon Footprint” NPG. However, in addition to use of bio-based raw materials and renewable energy, the NPG product’s relative sustainability and carbon footprint will result from your team’s ability to optimize process energy consumption and incorporate reliable renewable energy-based utility systems to power the process and equipment systems.

The project’s business objective is to design a new world scale 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, with solid flakes packaged in 1 MT supersacks. Current market pricing is to be expected for NPG product(s), raw materials, and utilities. Although a peer reviewed Life Cycle Analysis (LCA) is necessary to backup “Net Zero Carbon Footprint” marketing claims, an internal screening LCA is sufficient to confirm whether the NPG product will meet the “Low Carbon Footprint” or “Net Zero Carbon Footprint” targets.

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 production facility 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.

References

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5. BTX Produced from CO_2

(Recommended by Dimitris Collias, Penn; Proctor & Gamble (retired); Aeiforia Innovations LLC)

Background

BTX is a mixture of benzene, toluene, and mixed xylenes (para-, meta-, and ortho-xylene) and these chemicals are 3 of the 7 primary chemicals of the Chemical Industry (the other 4 primary chemicals are ethylene, propylene, ammonia, and methanol). In 2022, BTX global use was 129 million tonnes and its market size was $146 billion (Statista.com). Major uses of BTX chemicals are in polystyrene (PS); Nylon 6 and 6,6; polycarbonates; epoxy resins; poly(ethylene terephthalate) (PET) for bottles, films, and fibers; paints; surfactants; and disinfectants (see below). Fossil-derived BTX is currently produced via steam cracking or catalytic reforming of naphtha.

Based on the UN, keeping the global average temperature increase at 1.5°C maximum by the end of the 21st century would require net zero greenhouse gas (GHG) emissions (NZE) by 2050. In turn, that would require commercialization of technologies with either reduced-, zero-, or negative-emissions, as pledged by over 50% of the world's 2000 largest public companies and countries representing at least 88% of GHG emissions.

CO_2 is the feedstock that could be catalytically converted / aromatized to BTX, which can have negative GHG emissions. In this case, CO_2 can come from either Direct Air Capture (DAC) or point-source (e.g. smokestack) capture. Two potential routes of CO_2 aromatization via hydrogenation and acid catalysis (both requiring H_2) are shown in the schematic below (Fig. 1 from the article: doi.org/10.1016/j.jcou.2020.101405; RWGS and FT are the commercialized Reverse Water Gas Shift and Fischer-Tropsch processes, respectively).

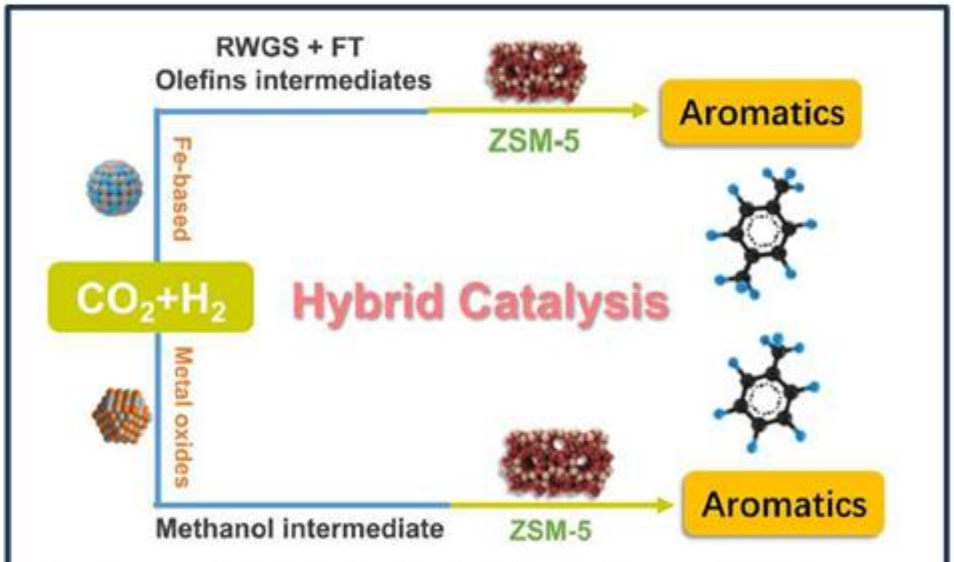


Fig. 1. Two typical routes developed for direct CO_2 aromatization via combined CO_2 hydrogenation and acid catalysis.

Approach, Goal and Project Impact

Techno-economic assessment (TEA) and life-cycle assessment (LCA) are methodologies for assessing the economic and environmental impacts of a product including production, distribution, use, and end-of-life (EoL).

Calculate the total cost of manufacture and perform a profitability analysis of BTX produced from CO_2 via chemical conversion / aromatization. Also calculate the GHG emissions and perform a screening LCA.

If both the cost of manufacture and GHG emissions of BTX, produced from CO_2, are lower than those of fossil-derived BTX, then various companies will explore producing product and packaging materials with BTX from CO_2.

Project Scope and Deliverables

The envisioned project scope should include:

- Determination of reasonable process flow diagram (PFD) of CO_2 to BTX via literature / art search and selection of the most informed and established process
- You may select any plant capacity, considering economy of scale, maximum equipment dimensions, size of the market, feedstock availability, etc.
- Process modeling of the full process with energy and mass balances
- Development of TEA and LCA process models with minimum final deliverables of cost of manufacture and profitability analysis and GHG emissions of BTX, also considering valuable by products. Other LCA metrics should be included if time allows.
- Comparison to cost of manufacture and GHG emissions of fossil-derived BTX

References

doi.org/10.1016/j.jcou.2020.101405

6. BTX Produced from Plastic Waste and Biomass

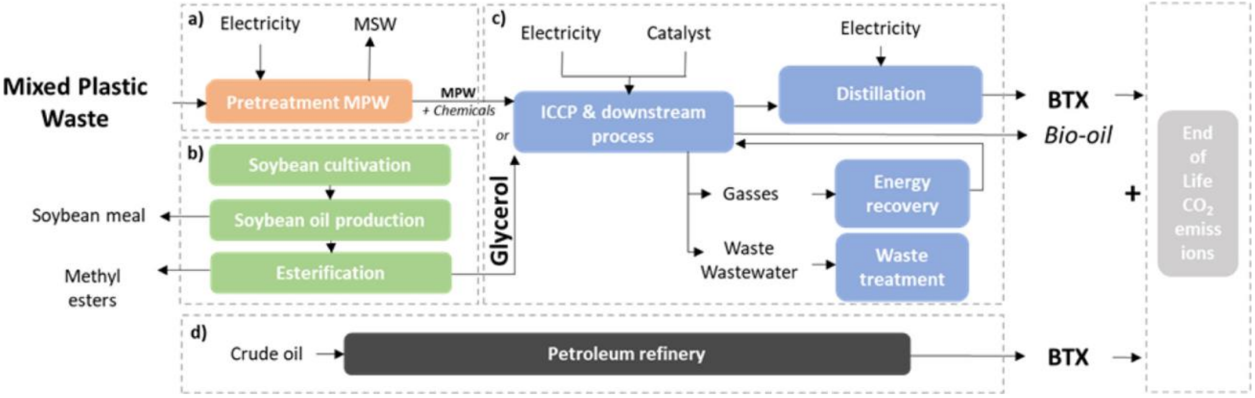
(Recommended by Dimitris Collias, Penn; Proctor & Gamble (retired); Aeiforia Innovations LLC)

Background

BTX is a mixture of benzene, toluene, and mixed xylenes (para-, meta-, and ortho-xylene) and these chemicals are 3 of the 7 primary chemicals of the Chemical Industry (the other 4 primary chemicals are ethylene, propylene, ammonia, and methanol). In 2022, BTX global use was 129 million tonnes and its market size was $146 billion (Statista.com). Major uses of BTX chemicals are in polystyrene (PS); Nylon 6 and 6,6; polycarbonates; epoxy resins; poly(ethylene terephthalate) (PET) for bottles, films, and fibers; paints; surfactants; and disinfectants (see below). Fossil-derived BTX is currently produced via steam cracking or catalytic reforming of naphtha.

Based on the UN, keeping the global average temperature increase at 1.5°C maximum by the end of the 21st century would require net zero greenhouse gas (GHG) emissions (NZE) by 2050. In turn, that would require commercialization of technologies with either reduced-, zero-, or negative-emissions, as pledged by over 50% of the world's 2000 largest public companies and countries representing at least 88% of GHG emissions.

Plastic waste and biomass could provide feedstocks (with almost zero and negative GHG emissions, respectively) for chemical processing. Anellotech (Plas-Tcat™ technology) in the US and BioBTX (Integrated Cascading Catalytic Pyrolysis technology; see Figure 1 below for its description from the article: doi.org/10.1021/acssuschemeng.3c06996) in the Netherlands are companies working on converting plastic waste and biomass to BTX.



Approach, Goal and Project Impact

Techno-economic assessment (TEA) and life-cycle assessment (LCA) are methodologies for assessing the economic and environmental impacts of a product including production, distribution, use, and end-of-life (EoL).

Calculate the total cost of manufacture and perform a profitability analysis of BTX produced from plastic waste and biomass (2 separate cases) via chemical conversion. Also confirm the GHG emissions from the reference and perform a screening LCA.

If both the cost of manufacture and GHG emissions of BTX, produced from plastic waste and biomass, are lower than those of fossil-derived BTX, then various companies will explore producing product and packaging materials with BTX from plastic waste and biomass.

Project Scope and Deliverables

The envisioned project scope should include:

- Determination of reasonable process flow diagram (PFD) of recycled plastics and biomass to BTX via literature / art search and selection of the most informed and established process
- You may select any plant capacity, considering economy of scale, maximum equipment dimensions, size of the market, feedstock availability, etc.
- Process modeling of the full process with energy and mass balances
- Development of TEA and simplified LCA process models with minimum final deliverables of cost of manufacture and profitability analysis and confirmation of reported GHG emissions of BTX, also considering valuable by products. Other LCA metrics should be included if time allows.
- Comparison to cost of manufacture and GHG emissions of fossil-derived BTX

References

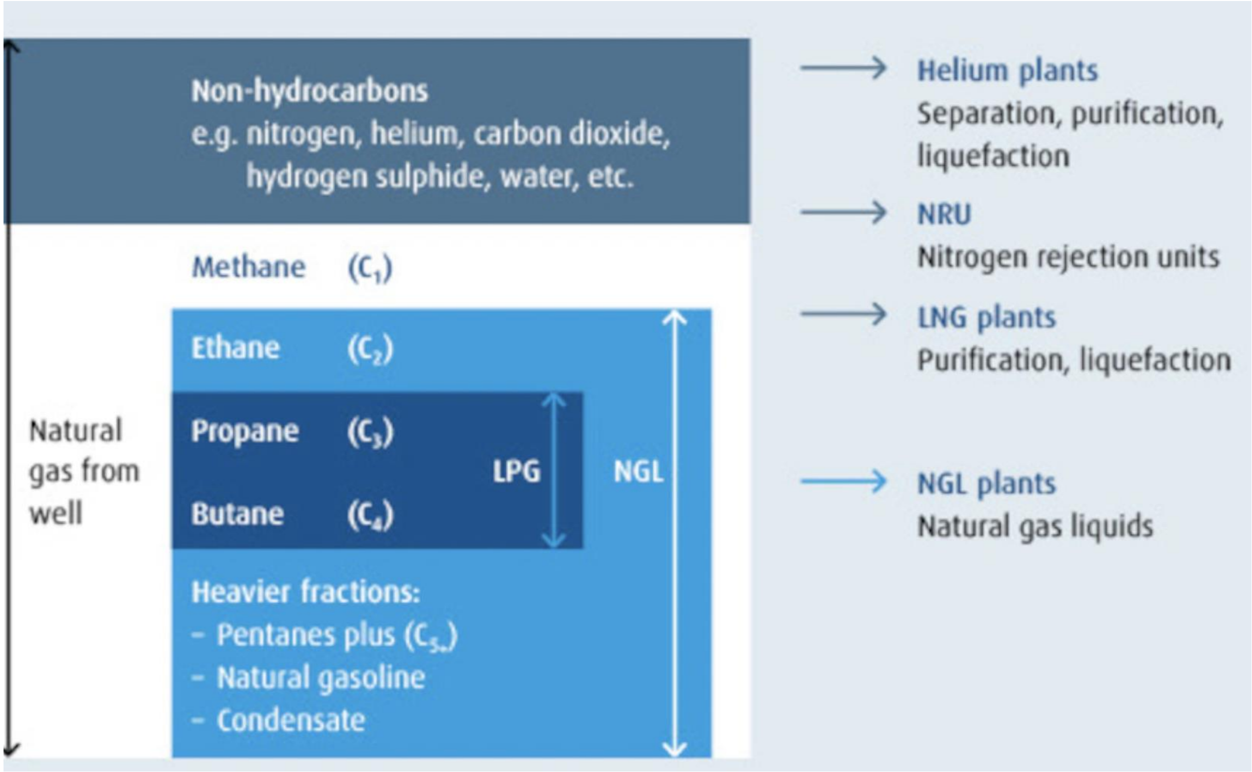
doi.org/10.1021/acssuschemeng.3c06996

7. Helium Liquification
(Recommended by Liang Dong and Alan Han, Penn)

Background

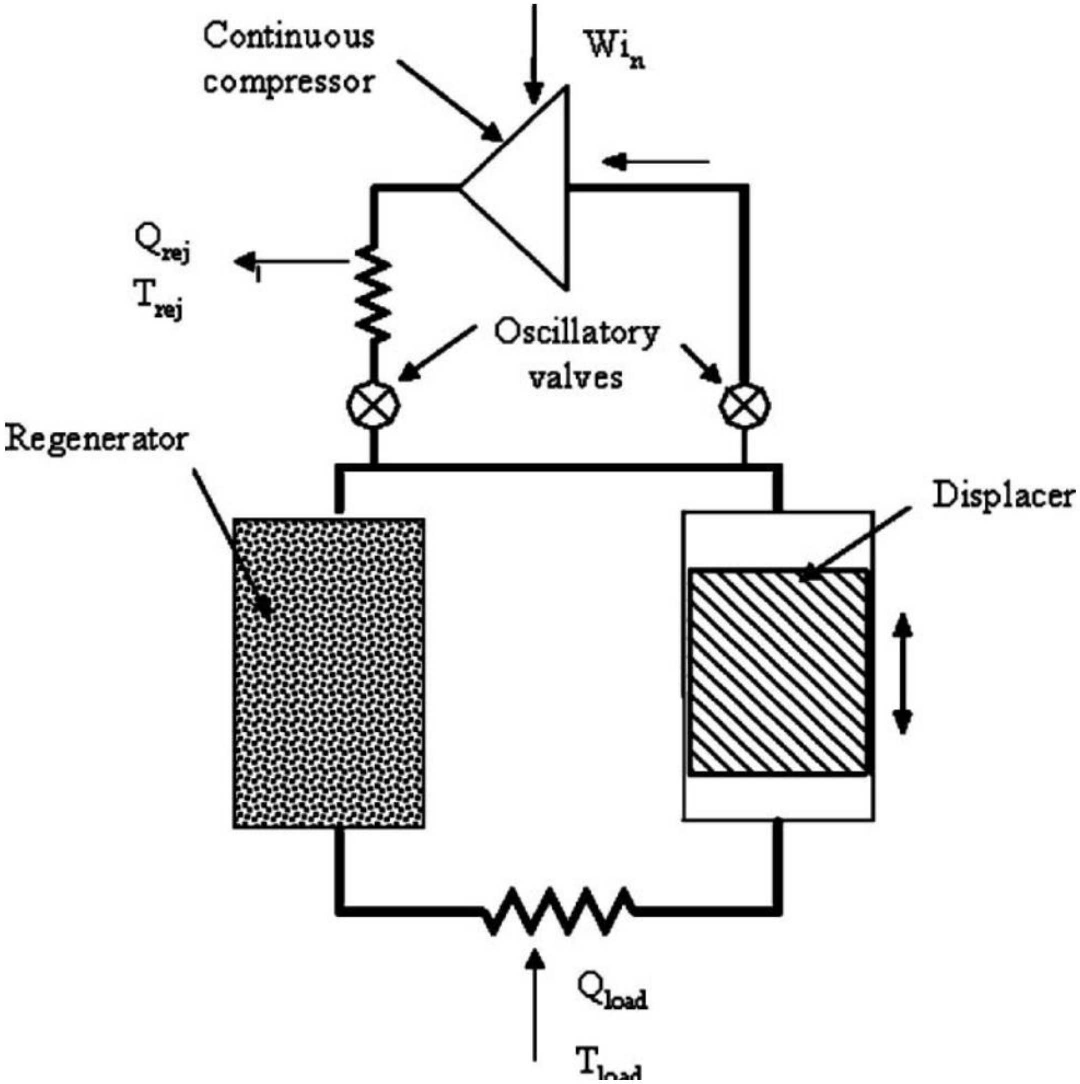
Cryogenics has always been a research-intensive area. Scientists still struggle to obtain very low temperatures for any chemical, including helium. At standard pressure, the temperature required to liquify helium is −269 °C. However, liquid helium is crucial for lab and hospital use, especially for instruments that operate at cryogenic temperatures. Helium is, of course, not a renewable resource (on Earth in less than geologic time scale).

Natural gas is an important source of clean energy and is crucial for many chemical processes. However, it must be processed before it can be used in applications. Usually, CO_2 is removed from the gas; natural gas liquids such as ethane, propane, and butane are recovered; and if He is present in the feed gas, it can be (but is not always) separated and purified as well. Nitrogen rejection is typically combined with the recovery of He.



The field of cryogenics is generally referred to as those processes that occur in the temperature range roughly T <120 K, where the permanent gases (nitrogen and oxygen) are condensed. However, Helium liquefies at a much lower temperature around T=4.2K. There are two forms of liquid He: He I and He II. He I is the normal liquid that has a critical point of T=5.2K and p= 0.227 MPa. He II is a type of superfluid (a quantum-mechanical state of matter) with a boiling point of T=2.2K and has much more interesting properties. Here we focus on He I.

The figure below shows a GM (Gifford-McMahon) cycle that is a type of regenerative cryocooler, which is different from recuperative cycle machines like Collins cycle. The fluid flows periodically within the machine and extracts heat from the lower end of the regenerator, which is similar to a heat exchanger but needs a large volumetric heat capacity. In the figure, Q_{load} is the heat exchanger where He is liquefied.



Problem Statement

Design a plant that can simultaneously remove CO_2 and nitrogen, recover natural gas liquids including ethane, propane, and butane, and liquefy and store helium. The feed stream you should process is from a newly discovered gas field, with production of 100 MMSCFD with a composition of:

65% methane
10% ethane
7% propane
6% butane
5.3% CO_2
4% nitrogen
2.7% He

Based on an annual gross processing of 53.3 billion cubic feet (Bcf) per day and 510 natural gas processing plants as of 2017 in the U.S., the average plant processes 34.25 cubic meters per second. You may assume that your plant has pipeline access for the feed natural gas and methane product, destined for an LNG terminal, and pipeline access for nitrogen (should you choose to compress and sell it). Because your feed is relatively impure, you can assume it is available to you for 10% less than the Henry Hub price, based on its higher heating value. It has already been treated to remove sulfur and mercury compounds. Your methane product can be compressed and sold at a price that is a function of its purity. Other products are sold at market prices.

Using the cryogenic plant above as a reference, is there a way to improve the helium liquefaction process? Remember He liquefaction requires extremely low temperature and high pressure.

Natural gas is a mixture of gases, with hydrocarbons being the main component. However, natural gas always contains nitrogen. Nitrogen lowers the heating value of natural gas, and thus the selling price, and increases transport volumes. Pipeline specifications for nitrogen vary. Typically, however, no more than 3–4% nitrogen is allowed in most specifications. Is there a way to increase nitrogen rejection and make it less than 1% in the final product? To a first approximation, assume the methane selling price can be described as (1.01 + (0.04 – volume fraction N_2)) * Henry Hub.

Propane and butane recovery rate should be at least 99%.

Assume the pre-treatment of natural gas is done before entering this plant. This includes the removal of Hg and H_2S and necessary drying process to remove most of the water. The typical specification for water in natural gas has a dewpoint of -15°C, or about 33 ppm. Ice (from water or CO_2) is a problem in low temperature processes, as it fouls heat exchangers.

Estimate the economics (NPV and IRR) of your design as a function of natural gas price, which impacts the spread between your feed and product price. Test the sensitivity over a range of historic prices for all materials. You should consider whether your design changes over some reasonable range of prices of feed and all products. For example, it may not be economically attractive to remove nitrogen if the natural gas price is below a certain value.

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Coproducts must meet market specifications and be sold at market prices, or a discount depending on quality. Waste streams from purges or other streams should be identified with appropriate treatment before release to the environment. Since your main product is energy, your plant 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.

8. Electrochemical Liquid-Liquid Extraction for Gold Recycling (Recommended by Lily Min and Emma Dreispiel, Penn)

Background

The United States is one of the largest gold mining countries in the world, producing 172.7 tonnes of gold in 2023 [2]. 5% of the gold consumed worldwide was in electrical and electronics, and gold also plays an important role in space exploration by protecting satellites from solar radiation [3, 4]. However, current hardrock mining techniques pose environmental risks due to hazardous chemical separation processes. Surface mining for gold has also led to deforestation in tropical regions [6]. An environmentally friendly process for recovering gold from waste and landfills is necessary to offset the environmental damage caused by years of gold mining.

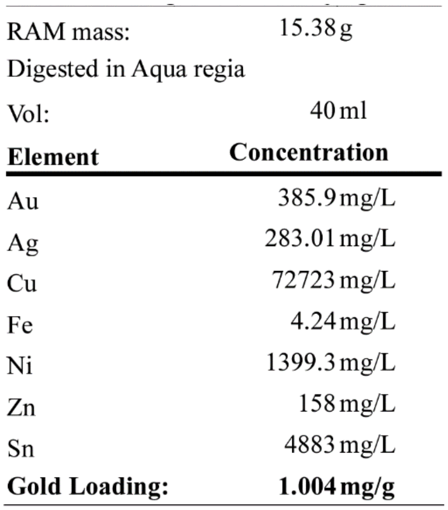
Current gold extraction techniques include carbon-in-leach (CIL) or carbon-in-pulp (CIP) processes. These use cyanide to form a gold-cyanide complex, which is extracted from a slurry through adsorption onto activated carbon [8]. However, since these processes require the recovery of activated carbon, they are not continuous. Other processes include electrode-based adsorbent systems, showing promise in metal leaching from electronic waste and mining streams. But these are not continuous processes either, requiring electrode regeneration to release the target species [10]. Thus, a continuous electrochemical separation process for precious metal recovery is necessary to better accommodate industrial-scale metal waste via improved sustainability and lowered operating costs.

One technique showing promise in precious metal recovery is selective ion capture, which is achieved by coating electrodes with redox-active materials. Polyvinyl ferrocene (PVF) electrodes can enhance the recycling of precious metals without destruction of the active catalyst structure. These units demonstrated a high affinity for ionic gold complexes, which can lead to gold purification at low energy costs. Additionally, liquid-liquid extraction (LLE) approaches using complex extractants have successfully recovered precious metals from aqueous phases, but the stripping process to recover the metals is slow and relies on wasteful thermal swings. Thus, electrochemical LLE (e-LLE) is explored as an enhancement to the precious metal recovery process.

Problem Statement

A recent paper in *Nature Chemical Engineering* proposes a novel, continuous, redox-mediated electrochemical liquid-liquid extraction (e-LLE) process for gold recovery from waste materials [10]. At the lab scale, they demonstrate a successful system using 1,1′-didodecylferrocene (ddFc), a redox extractant that has a high affinity to gold and platinum group metals. They highlight the “highly scalable and adaptable” potential of this work to be used in the future.

Your task is to scale this e-LLE process up to process a feed of 12,480 tonnes of electronic waste (e-waste) annually. This number comes from the UN’s estimate of 7.8 kg of e-waste per person per year, and a population of about 1.6 million people in Philadelphia [11,12]. You can assume that the e-waste is in the form of RAM chips, and the composition of a common RAM chip is listed in the table below [13]. You can assume the chips have already been digested/leeched and are entering the process in a slurry. You will need to decide on an appropriate market price to pay for this leachate, based on market information you may be able to find or by estimating the cost that a supplier would incur, including reasonable profit based on the capital required. For the leaching process, you will want to scale the following lab-scale feed: 150 g of Samsung RAM modules in 500 mL of 10mM KCN leach solution [13].



RAM mass: 15.38 g
Digested in Aqua regia
Vol: 40 ml

Element	**Concentration**
Au	385.9 mg/L
Ag	283.01 mg/L
Cu	72723 mg/L
Fe	4.24 mg/L
Ni	1399.3 mg/L
Zn	158 mg/L
Sn	4883 mg/L
Gold Loading:	**1.004 mg/g**

Figure 1. Samsung DDR2 RAM chip composition [13].

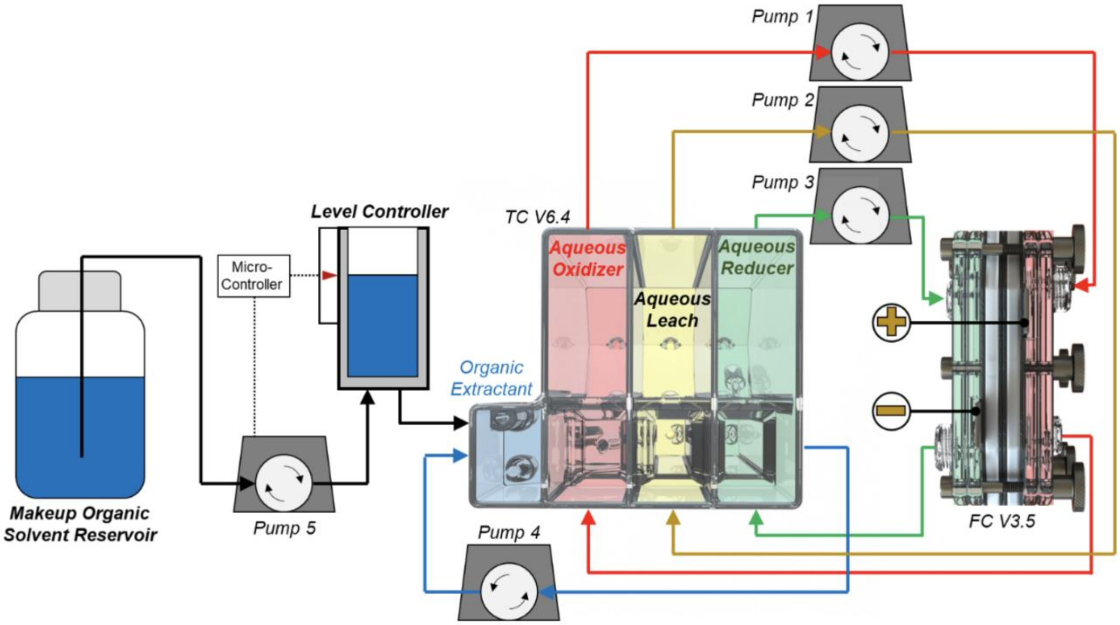


Figure 2. Schematic diagram of continuous e-LLE apparatus [10].

The basis of this process is a three-column extraction apparatus. The equations for each of the extraction columns are as follows:

1. The oxidation column
    a. ddFc extractant is activated by oxidation with an aqueous oxidizing agent
        i. $(½)\ I_3^- + \text{ddFc} \rightarrow (3/2)\ I^- + \text{ddFc}^+$ (from Figure 3 and 4)

2. The leaching column
    a. Aqueous gold-containing leach contacts the oxidized ddFc
        i. $\text{ddFc}^+ + (\text{Au(CN)}_2^-) \rightarrow \text{ddFc}^+\text{Au(CN)}_2^-$ (from Figure 3 and 4)
    b. The Elsner equation governs the leaching of gold with a cyanide complex:
        i. $4\ \text{Au} + 8\ \text{KCN} + O_2 + 2\ H_2O \rightarrow 4\ \text{K[Au(CN)}_2] + 4\ \text{KOH}$

3. The reduction column
    a. The gold is released. The dicyanoaurate is liberated through a reduction of $ddFc^+$ to ddFc with ferrocyanide as a reducing agent
        i. $ddFc^+ Au(CN)_2^- + Fe(CN)_6^{4-} \rightarrow ddFc + Au(CN)_2^- + Fe(CN)_6^{3-}$ (from Figure 3 and 4)

After the gold is released in the reduction column, pure gold is recovered through electrowinning.

Note that while KCN is mentioned as feed here and in the work to date, you should also consider modeling the process with the less expensive NaCN that is standard in typical gold extraction processes. You should quantify the economic benefit of using NaCN and KCN, while determining if the change in solvent alters the process efficiency. You also may want to study any useful coproducts, such as iodide, from the oxidation column.

Ultimately, the goal is to produce a design to recover gold from the e-waste leachate stream identified above and estimate the capital and operating costs. You should calculate the economics (NPV and IRR) as a function of the gold price, compared to the range of gold prices over at least the past two decades, to determine whether you recommend building the plant.

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Coproducts must meet market specifications and be sold at market prices, or a discount depending on quality. Waste streams from purges or other streams should be identified with appropriate treatment, particularly for cyanide wastes, before release into the environment. 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.

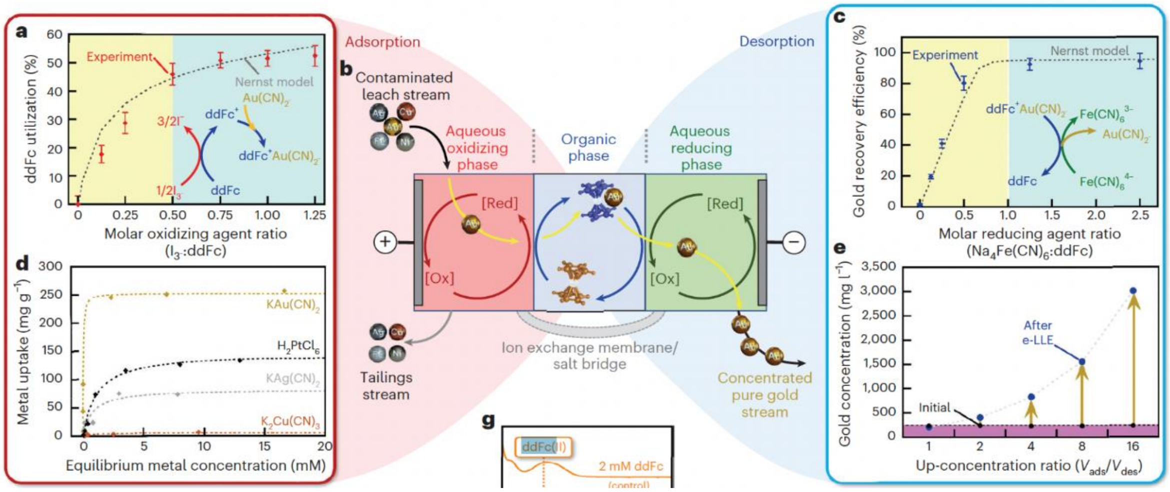


Figure 3. Schematic of the reaction process between extraction columns 1-3 [10].

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9. Sustainable Lithium-ion Battery Recycling via Hydrometallurgical Approaches (Recommended by Sara Takenaka and Nicole Zhao, Penn)

Background

The use of lithium-ion batteries is widely prevalent in powering consumer electronics, automotive, and large-scale energy storage applications. Soaring demand for lithium-ion batteries in emerging industries (like electric vehicles) has also introduced a variety of environmental concerns. Key materials like lithium and cobalt are not only labor and energy intensive, but they also generate considerable amounts of pollution. Their short device lifetime results in tens of thousands of tonnes of lithium batteries disposed of annually. Despite this, only an estimated 5% of lithium batteries are recycled.

Lithium batteries contain a valuable amount of materials: lithium, cobalt, graphite, copper, nickel, aluminum, manganese, etc, which can produce millions in dollars of residual value. However, lithium battery recycling still faces many challenges in terms of technical constraints, economic barriers, logistic issues, and regulatory gaps.

Problem Statement

A major automotive manufacturer is seeking a partnership to recycle the lithium-ion batteries in their retired electric vehicle fleet, and Li-recycle is interested in the project. However, they will need to significantly scale up their process to be competitive. The largest plant in operation can handle a volume of 10,000 tons/year; the auto manufacturer hopes to build a plant with a 100,000 ton annual capacity.

There are a variety of methods used currently to recycle lithium batteries. Your task is to design a hydrometallurgical method to recover lithium ion materials from black mass (a component of lithium batteries that consists of cathode and/or anode electrode powders). The black mass will consist of lithium metal oxides, lithium iron phosphate (cathode material), and graphite (anode material).

A process flow diagram of a suggested process is shown below in Figure 1.

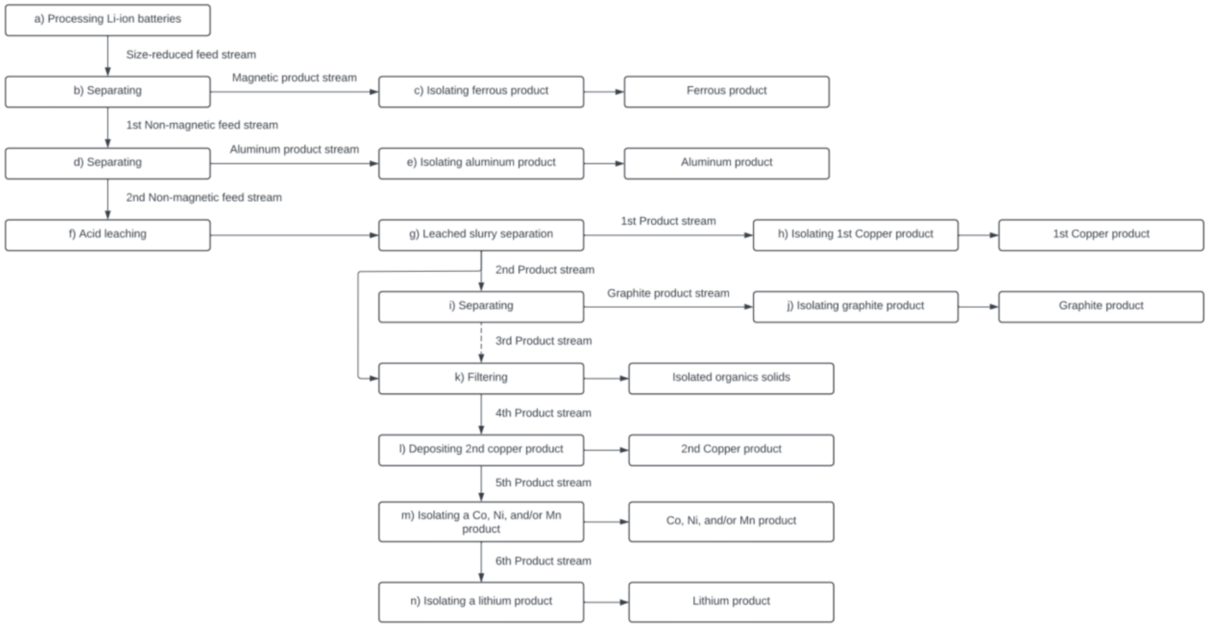


Figure 1: Process Flow Diagram

Your team has been tasked with demonstrating the feasibility of the project and important techno-economic considerations in deciding whether to pursue this venture. The following deliverables are expected:

Part 1: Process Requirements
Start by preparing a detailed material balance and process flow diagram for a system that can handle a volume of 100,000 tons/year. Assume that the plant runs continuously for 48 weeks in a year; the remaining days include the startup, shut down, and maintenance time required.

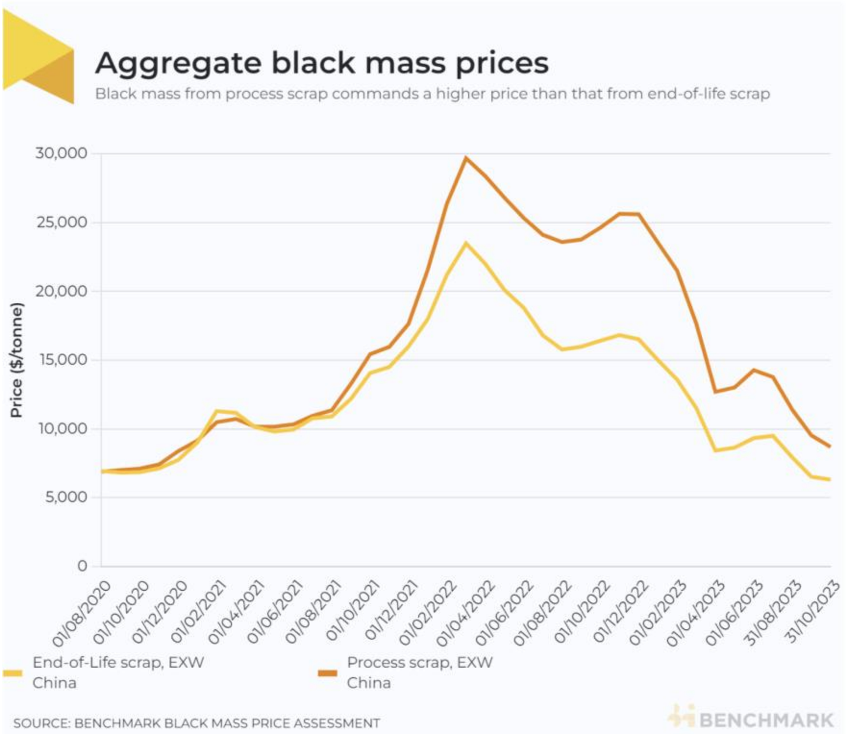
Part 2: Equipment Requirements
Identify the necessary equipment for the process based on the material balance. Include equipment size, a ranked list of 2-3 options for manufacturers, and the projected capital cost for the project.

Part 3: Electricity Consumption
Calculate the electricity consumption per ton of black mass processed based on the equipment requirements. Use this value to calculate the annual electricity consumption for the process and the cost of electricity used for this process, using historical pricing data. Assume the plant will be located in Texas, near the auto manufacturer's biggest facility.

Part 4: Economic Analysis
Analyze the necessary capital and operating costs and profitability of the project (NPV and IRR) over the next 5 and 10 years. Identify the breakeven point for the project and potential risks that could impact the outcome of the economic viability of the project (e.g. natural disasters, significant changes in demand for recycled lithium). You can assume that the cost to disassemble and shred the batteries to produce your feed stream is $10,000/tonne of black mass (Figure 2).

Part 5: Life-cycle Analysis
Determine the sustainability of the project relative to lithium mining. Consider greenhouse gas emissions, potential socioeconomic changes (e.g. increase/decrease in jobs), and direct environmental impacts.

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Coproducts must meet market specifications and be sold at market prices, or a discount depending on quality. Waste streams from purges or other streams should be identified with appropriate treatment before release to the environment. Energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Fully document your assumptions in your analysis.



SOURCE: BENCHMARK BLACK MASS PRICE ASSESSMENT

Figure 2: Aggregate Black Mass Prices

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