Suggested CBE 459 Design Projects – 2020-2021

1. Biofuels for Aviation
(Recommended by Rick Bockrath, Consultant – retired from DuPont)

Background

You are the Senior Vice-President for Sustainability at one of the largest Airline carriers. The current core sustainability goals for your company are heavily focused on the improvement of the fuel efficiency of the jet engines and increasingly sophisticated AI-based management of the routes taken by the planes to minimize fuel consumption. There has been a consistent desire to have a third focus by moving into sustainable, bio-based fuels. Yet so far, this has not been a viable commercial option. Aside from some clearly press release-oriented activities, there has been no clear-cut movement toward such sustainable fuels because of their apparently high cost structure.

Gevo is the company that seems to be the furthest along in developing such a biofuel. In December 2019 they released a "White Paper" document entitled "SUSTAINABLE AVIATION FUEL: Alcohol-to-Jet Synthetic Paraffinic Kerosene Is a Proven Pathway to Deliver a Bio-Based, Low-Carbon Option to Travelers". The following statement in the document summarizes the current dilemma:

"… the cost of producing biojet is estimated to be two to seven times greater than conventional jet fuel for the foreseeable future".

Your fear is that "seven times greater" is more likely than "two times greater".

Gevo's overall transformation technology is based on fermentation of corn mash directly to isobutanol followed by dehydration of isobutanol to isobutene which is then oligomerized to an isoparaffinic mix that is about twelve carbons in length, which is a good jet fuel. Gevo has extensively tested their material, which is called ATJ-SPK against Jet Fuel standards (ASTM D1655/7566) and has shown that it meets the required specifications.

The key to any biofuel will be a highly scalable series of unit operations from initial feedstock through final product. This is especially critical for the large volume production of jet fuels. Your company hired an outside technology assessment firm to look at the Gevo process and their key conclusions are given below:

a) The concept of retrofitting US ethanol plants to make isobutanol instead of ethanol is of interest since US ethanol plants are world scale and consistent with bio-fuel volume needs.
b) The dehydration of isobutanol to isobutene is well established technology that is commercially practiced, and the technology is available for licensing from a number of technology providers. Yield is virtually 100%.
c) The oligomerization of isobutene (C4) to an average chain length of twelve is a quite reasonable extension of well-known isooctane (C8) technology which is widely practiced commercially and is available from a number of technology providers. Yield is virtually 100%.
d) The key bottleneck in the overall process is that the retrofit of an ethanol plant to make isobutanol appears to result in a dramatic decrease in overall plant capacity. The plant capacity is no longer world scale. This has the result of making the isobutanol generation step very expensive.
e) To make the corn to isobutanol to biofuel process sequence viable, an alternative way to make isobutanol is needed.

f) Since ethanol plants are highly efficient in making ethanol, a potential route to isobutanol via ethanol and methanol could be quite advantageous and might make the overall corn to bio-fuel story successful. The chemistry involved is called Guerbet chemistry. The overall sequence would then be:

Corn mash to ethanol.
Ethanol and biomethanol to isobutanol.
Well established technologies for the dehydration and oligomerization steps.

Since your company's expertise is neither in chemistry nor catalysis, you contracted with a group of academic/industrial consultants in this field to fully explore the Guerbet chemistry technology landscape for cost efficient transformations. They found the following article to be the most promising; although, it must be realized that the work is at the early stages of R&D development.

"Higher-Alcohols Biorefinery: Improvement of Catalyst for Ethanol Conversion", E. S. Olson, R. K. Sharma and T. R. Aulich, Applied Biochemistry and Biotechnology Vol. 113–116, p 913- 933, 2004

In the article, isobutanol is the dominant product at 90+% yields. Biomethanol can be made from biomethane which can be obtained from a number of different sources. Bioethanol is readily available from current ethanol plants.

The improvements detailed in the article are significant enough to justify further analysis. If the analysis is positive; then, upper management will likely want to approach the owner of the technology to discuss a joint development R&D partnership.

Since the technology is in its early R&D stage, the consultants suggest that the following assumptions be used in the analysis.

a) It is likely that the catalyst activity can be markedly improved and so a rate that is three times higher than the results in Table 4 (Ni-FM case) is reasonable.
b) The product distribution will be more difficult to improve on and so assume the product mix from Table 4 (Ni-FM) for the liquid compounds and Table 3 for the gases for the analysis.
c) The authors demonstrated the successful recycle of the lighter alcohols to the desired product and this should be assumed in the analysis.
d) Catalyst decay rates are not provided. They suggested that you oversize the reactor bed by 50% over the (kg of product/hr)/(kg of catalyst) demonstrated in Table 4. It should be noted that the conversion of the ethanol was 100% and so the flow rate through the reactor could have been higher while still getting very high conversions. Therefore using 100% conversion rate data plus a further 50% increase allows for significant activity decay before the bed must be renewed.
e) Assume the bed has a 2-month life before it must be decoked.
f) Since the support is activated carbon there will be some loss of catalyst in the decoking step. Assume that there is a 10% catalyst loss that must be made up by the addition of fresh catalyst to the top of the bed.
g) The catalyst uses inexpensive metals and salts and is not expected to be expensive. They suggest assuming $5/lb for the Ni-FM catalyst. This is approximately 25% higher pricing than Fluid Cat Cracker catalyst.

You need a technoeconomic analysis of the overall cost of transformation. You do not want the cost of purchasing bioethanol or biomethanol to confuse the initial analysis, so your focus is on the

transformation cost. You have started discussions with your Logistics/Supply organization to answer those feedstock cost questions. This analysis is to focus on the CAPEX and OPEX to take ethanol and methanol through to biofuel. You have had preliminary discussions with the current technology providers for the dehydration and oligomerization steps at the scale of interest to you and so the analysis is to assume the following:

Dehydration step: CAPEX of $ 0.10/kg/yr of jet fuel, OPEX of $0.03/kg of jet fuel. 100% yield

Oligomerization step: CAPEX of $ 0.15/kg/yr. OPEX of $0.034/kg of jet fuel. 100% yield

Once you have an analysis of the ethanol/methanol to isobutanol step's CAPEX and OPEX, you can then bring all of the transformation steps together and have an overall picture of the process cost structure.

For this analysis assume the plant capacity is 100 kt/yr jet-fuel (129 kiloton isobutanol).

As a framework for comparison, your company pays close attention to the cost difference between crude oil and jet fuel. Over the 2010 to 2019 time period, the spread has averaged $0.05/kg of jet fuel. Clearly the existing cost of transformation is quite efficient. This spread covers OPEX and a return on the CAPEX. You realize that bio-jet will be more expensive than regular jet fuel, but it is unlikely that you can "afford" more than a $0.50/kg cost of transformation OPEX and return on CAPEX. Your goal is to find out if this can be achieved.

You will need to make many assumptions in the course of completing the analysis and so management will expect a strongly positive result before proceeding further due to the uncertainties inherent in your analysis. An IRR of greater 20% should be sufficient. You expect that you will exceed 20% but if your analysis falls short then upper management wants to know the required price to reach 20%.

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. You will need to make many assumptions and these need to be fully documented in your analysis.

References

"Higher-Alcohols Biorefinery: Improvement of Catalyst for Ethanol Conversion", E. S. Olson, R. K. Sharma and T. R. Aulich, Applied Biochemistry and Biotechnology Vol. 113–116, p 913- 933, 2004

" SUSTAINABLE AVIATION FUEL: Alcohol-to-Jet Synthetic Paraffinic Kerosene Is a Proven Pathway to Deliver a Bio-Based, Low-Carbon Option to Travelers", GEVO White Paper, December 2019.

2. Protein Purification to Produce Edible Soybean Protein (Recommended by P. C. Gopalratnam, Consultant – formerly DuPont, INVISTA)

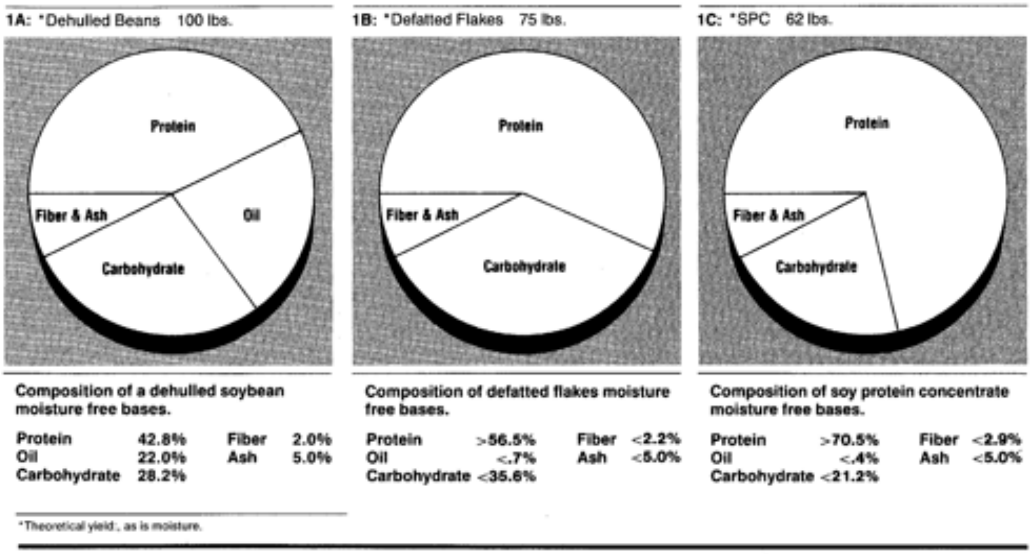
Introduction

Soybean meal (the physical form is flakes) is the residual material remaining after oil has been extracted from soybeans. It is a product relatively high in protein, and has long been used for animal feed, but because of flavor and texture problems, has not been widely used in human foods. However, a process has been developed which uses alcohol extraction to render the meat palatable.

The soy is first defatted using Hexane prior to the protein extraction step. With an aqueous alcohol wash process the sugars are dissolved with alcohols (methanol, ethanol or isopropyl alcohol) in a batch or a continuous process. These alcohols do not dissolve the soy proteins. After the extraction of the sugars, the alcohol is recovered and re-used through partial separation of Ethanol-H_2O stream from the Carbohydrates. The recovery is achieved by evaporation and a distillation/stripping column.

The composition of soybean solids after flaking in preparation for oil extraction is given in Figure 1-A. After the oil has been extracted with hexane and the flakes have been dried the composition is that given in Figure 1-B. The de-oiled flakes can be made suitable for human consumption by using a proprietary ethanol extraction process which removes carbohydrates and soluble residues along with objectionable flavors, to yield a nearly bland (flavorless) soy protein concentration (SPC) product of the composition given in Figure 1-C.

FIGURE 1. Protein Concentration Process



Composition of a dehulled soybean moisture free bases.			
Protein	42.8%	Fiber	2.0%
Oil	22.0%	Ash	5.0%
Carbohydrate	28.2%		

Composition of defatted flakes moisture free bases.			
Protein	>56.5%	Fiber	<2.2%
Oil	<.7%	Ash	<5.0%
Carbohydrate	<35.6%		

Composition of soy protein concentrate moisture free bases.			
Protein	>70.5%	Fiber	<2.9%
Oil	<.4%	Ash	<5.0%
Carbohydrate	<21.2%		

*Theoretical yield., as is moisture.

Solids containing mainly proteins flakes and insoluble carbohydrates are then dispersed in water, neutralized to pH 7.0 if necessary, and spray-dried with hot air to produce soy concentrates.

Problem Statement

You are an engineer in the Protein Power Division of an Agricultural Processing Corporation, a firm that processes agricultural products. As a member of the Corporate Engineering Department, your assignment is to complete a preliminary design and economic analysis of a new soy protein concentrate facility using an aqueous ethanol (60-80%) extraction process, which their R&D has developed. The starting material for

your project is dried de-hulled soybeans, which must be defatted by removing fat and oils with hexane and dried prior to the protein extraction process as shown in Figure 1. The new facility will be built near Decatur, Illinois.

Soy proteins appear to be least soluble in about 50% aqueous alcohol; their solubility increases on either side of that concentration. The preferred alcohol concentration in the protein extraction step is 60% by weight. Excess water in the extraction solvent is to be avoided because of additional energy costs for removal and because an extremely wet soy protein cake tends to agglomerate, clogging the process system. The aqueous alcohol (up to 10% water by weight) removed from the alcohol water soy solubles is recycled to the extraction step.

Following the completion of pilot plant studies, a semiworks operation with a capacity of 680 lbs product/ hour was started up. The market has now been developed to the point that the construction of a 50 MM lb/yr facility on a dry basis (solid phase) is being investigated. The pilot plant data indicates suggested solids to aqueous alcohol ratio of approximately10% in the extractor and a recycle that needs about 10% fresh alcohol makeup.

The pilot plant was run at a feed temperature of about 80° F and the extraction was performed around 140° F. While the pressure and temperature of these streams may be used from the semiworks, the scale up should be redesigned to find the economic optimum since the semiworks was built as part of a feasibility study, probably inefficiently. Explore process alternatives such as batch vs. continuous protein extraction vessel and distillation internals like sieve tray, bubble cap or structured packing for efficiency. Assume a plant uptime of 85% for this facility.

Safety may also play a key role in finding an economic optimum on an NPV basis and if the concentration of alcohol in air in the flash dryer exceeds the explosive range, process alternatives as well as waste water treatment will have to be evaluated resulting in possible increased capital costs.

The finished edible product will be conveyed across the fence to the silos in their packaging facility next door. Your marketing people want the selling price of the edible soy protein product necessary to achieve the corporate hurdle rate of 15 % IRR for the 50 MM lb/year project.

References

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- Null, H.R., Phase Equilibria in Process Design, Wiley-Interscience, New York (1970).

3. Design of COVID-19 Vaccine Production Process (Recommended by Jeffrey D. Cohen, Janssen R&D)

Historically, large-scale influenza vaccine production has employed inoculating embryonic chicken eggs with the genetic composition indicative of the infectious species [1,2,3]. A global pandemic, on the scale of COVID-19, may require billions of individual vaccine doses. A step-change increase in the classic, vaccine-production process, i.e. an increase in the volumetric productivity of the active pharmaceutical ingredient (API) versus the legacy process, is required to meet the need of the global population.

Making a vaccine against the coronavirus that causes COVID-19 involves a variety of technologies and approaches. As it's unclear which technology will be best, scientists must develop multiple routes simultaneously.

With any vaccine, the aim is to get the body's immune system to recognize a specific pathogen [4]. Once recognized, the immune system develops agents poised to attack if that pathogen should appear again during an infection. The objective is to protect people from getting sick if exposed; or, at a minimum avoid severe illness.

The Chinese government publicly released the genetic sequence of the virus that causes COVID-19, called SARS-CoV-2, in mid-January, just a few weeks after recognizing an outbreak was underway. The move immediately triggered a flurry of vaccine development projects.

Getting the sequence meant developers could begin going after what they knew would be the key target: the so-called spike protein found on the surface of SARS-CoV-2, which gives it its distinctive profile.

One of the challenges now is that scientists still don't know much about what the virus does to the immune system. They are designing a vaccine without knowing how long its benefits will last or what level of immune response they need to generate.

Vaccines often take 15 to 20 years to develop. Researchers are trying now to develop a SARS-CoV-2 vaccine in just a year to 18 months. To meet this tight deadline, scientists are trying new vaccine technologies under development for years, but have not been used to treat large populations.

At a time when the world is waiting for a vaccine, technologies with the longest track record – yet take the longest to produce – might not be the winning approach. Newer, faster techniques must prove they can be made safe, effective and at a scale sufficient to make a difference.

Below is a list of various technologies employed in the development of a potentially-effective vaccine, with an abridged list of pros and cons [5,6]:

- **Whole virus vaccine: Live-attenuated**
    - **Strengths:** Used for decades in billions of children, safe and effective, for example, in combating measles, mumps and rubella in a combined shot.
    - **Weaknesses:** Theoretically, these vaccines also can cause the disease they were designed to prevent. Can also take years to formulate, challenge of finding balance of safety and efficacy– ensuring the virus is sufficiently weakened to be safe, yet powerful enough to trigger an effective immune response.

- **Whole virus vaccine: Inactivated**
    - **Strengths:** The inactivated form of whole virus vaccines is considered safe as it cannot cause the illness it is designed to protect against.

    - **Weaknesses:** Can worsen symptoms in some patients who catch the virus. Potentially dependent upon method used to inactivate the virus.

- **Protein-based vaccine**
    - **Strengths:** Are relatively easy to manufacture, safe and proven to provide immune responses.
    - **Weaknesses:** To be effective, this vaccine may need to be paired with an immune stimulant, which can cause side effects.

- **Viral vector vaccines**
    - **Strengths:** Viruses are great at invading cells and using their machinery to make more copies of themselves. These vaccines can spur a strong immune response, likely to be effective.
    - **Weaknesses**: People may get mild, flu-like illness. Not advised for people who are immunocompromised.

- **Nucleic acid vaccines**
    - **Strengths:** Vaccine based on delivering strands of genetic material – essentially an instruction manual to turn people's cells into spike protein factories. These vaccines can be developed very quickly. Technology may be based on RNA, other nucleic acid candidate vaccines use double-stranded DNA, which is more stable. Once inside the person's cells, this is translated into mRNA and then makes the spike protein.
    - **Weaknesses:** This novel approach to vaccine development has never been tried before in large numbers of people, so there are lots of open questions about its safety and effectiveness. A second dose probably will be needed for the body to mount an adequate immune response. Frequent boosters could be needed later if immunity is not long-lived. Since nucleic acid vaccines have never been manufactured before at a scale larger than a clinical trial, there is some concern it will be difficult to manufacture enough to make a difference in the global pandemic. But Moderna has said it will be able to make between 500 million and 1 billion doses per year by next year.

In recent years the utilization of genetically-engineered, animal cells, grown in production-scale bioreactors, subsequently transfected with viral-related, genetic material, has shown promise in producing a sufficient mass of vaccine-API to meet the estimated global need.

The objective of this project is to select a biocatalytic technology, potentially from the list above, and design an upstream and downstream manufacturing process, i.e.:

- an initial series of bioreactors to expand the cellular-biocatalyst population, subsequently transfected with viral material, responsible for API production, followed by
- the unit operations needed to isolate, purify, and package the bulk API, for subsequent packaging into individual doses.
- estimate capital investment and operating cost to produce 500 million doses of API for a COVID-19 vaccine [7].
    - Note: due to the urgency of medical need, the process you specify will inform your search for a suitable contract manufacturing organization with the appropriate equipment

already installed. The economic analysis will enable negotiating the CMO manufacturing costs.

References

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2. S. Wong, R.J. Webby, Traditional and New Influenza Vaccines, Clinical Microbiology Reviews, p. 476–492, July 2013 Volume 26 Number 3, https://www.cdc.gov/flu/prevent/how-fluvaccine-made.htm
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4. Carbon Dioxide to p-Xylene (Recommended by Gary Sawyer, CDI Corporation)

With carbon capture technologies improving and the need for fixing carbon ever rising, new and novel chemistries are advancing to convert carbon dioxide to higher value chemical products and intermediates. When combined with clean hydrogen from, for example, water hydrolysis using wind energy, then these new technologies would have a negative carbon footprint. In fact, a team of Japanese industry and academic institutions are investing roughly $20 million to advance the conversion of carbon dioxide to aromatics, particularly p-Xylene. p-Xylene is $50 billion/yr business . It is an important intermediate to polyethylene terephthalate (PET) plastic, most commonly found in soda bottles.

One group of researchers found catalysts that could convert up to 20% of the CO_2 per pass with selectivity to p-Xylene of around 40% at reaction conditions of 350 C, 3 MPa, and roughly 3:1 molar H2 : CO_2. Another group claims up to 40% CO_2 conversion with 75% selectivity to aromatics at similar reaction conditions. Byproducts include paraffins and olefins up to carbon number 6 or so, and carbon monoxide.

Your project is to design a plant to produce 250 kTA of p-Xylene (contained in mixed xylenes), based on the literature references provided. You can consider using the water gas shift reaction to convert byproduct CO to CO_2.

Battery limits are:

- Feeds:
  - Liquid CO_2 at 300 psig and -20 C
  - Hydrogen at 300 psig and 25 C

- Products:
  - Mixed xylenes (ortho, meta, para) at ambient temperature
  - Other aromatics (Benzene, toluene, ethylbenzene) at ambient temperature
  - Other liquid hydrocarbons at ambient temperature. Characterize their fuel value.
  - Other gases at standard conditions, to be used as fuel for the process as needed.

Your economic analysis should determine the prices for hydrogen and CO_2 that would provide a 10% return on capital (IRR), based on p-xylene at $0.50/lb. Provide some insight into current hydrogen production costs from water electrolysis based on your own literature search. Similarly, determine if a "green premium" is needed on the price of p-xylene to make investment worthwhile.

Siting considerations should include:

- Locations in the US with the highest renewable energy footprint
- Locations in the US with available CO_2, such as an existing pipeline . Calculate volumes of CO_2 that would need to be transported.
- Locations in the US where your products could most easily be shipped to customers.
- Availability of water for hydrogen generation.

Acknowledgement: Editorial advice and reference information provided by Professor Thomas Degnan of Notre Dame University is gratefully appreciated.

References

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4. Xu Cui, Peng Gao, Shenggang Li, Chengguang Yang, Ziyu Liu, Hui Wang, Liangshu Zhong, and Yuhan Sun, *Selective Production of Aromatics Directly from Carbon Dioxide Hydrogenation*, *ACS Catalysis* **2019** *9* (5), 3866-3876
5. If your site selection uses pipeline CO_2, use the conditions provided by the pipeline, typically over 1000 psig and ambient temperature.
6. See, for example, *A Review of the CO_2 Pipeline Infrastructure in the U.S.*, DOE/NETL-2014/1681, April 21, 2015.

5. RNA vaccine for Covid-19. Manufacture of 100 million sterile doses (Recommended by Dr. Scott L. Diamond, UPenn)

Delivery of mRNA to the cell surface for uptake is an example of transfection. The mRNA is combined with a lipid nanoparticle (LNP) containing cationic and neutral lipids and a PEGylated lipid. The mRNA-LNP formulation is taken up by the target cells, escapes the endosome into the cytoplasm where the mRNA is translated by ribosomes and the protein product is secreted or directed to the cell membrane. The immune response to the expressed protein should lead to the production of neutralizing antibodies (nAb) against the receptor binding domain (RBD) of SARS CoV-2 Spike (S) protein. Assume capability to make up to a 100 ug dose of mRNA per inoculation. Define a single dose or primer/booster strategy.

1. Identify the mRNA sequence that binds human ribosomes and leads to the expression of a protein that can provoke an immune response against the SARS CoV-2 spike RBD domain.

2. Define a mRNA synthesis and purification process using a DNA template, recombinant RNA polymerase and nucleotides for in vitro transcription of the RNA. Take special precautions to avoid RNases that degrade the mRNA product. Evaluate batch, CSTR, or PFR configurations. Address potential for recycle of RNA polymerase and unincorporated bases. Define QC metrics for mRNA product.

3. Define a LNP manufacturing synthesis and formulation process where lipid subcomponents and PEGylated lipids are synthesized and assembled into a narrow size distribution of lipid nanoparticles (LNP) ideal for formulation with mRNA for injection.

4. Measure bacterial and endotoxin levels for QC purposes for a sterile human injectable.

5. Determine the manufacturing cost per dose and evaluate the economics for $10 to $100 dose.

References

For >100 references, Pubmed search: lipid nanoparticle mRNA vaccine

Hassett KJ, Benenato KE, Jacquinet E, et al. Optimization of lipid nanoparticles for intramuscular administration of mRNA vaccines. Mol Ther Nucleic Acids 2019;15:1-11.

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Corbett KS, Flynn B, et al. Evaluation of the mRNA-1273 Vaccine against SARS-CoV-2 in Nonhuman Primates. N Engl J Med. 2020 Jul 28.

6. Ethyl Acetate With Ethanol Coproduct Option (Recommended by Leonard Fabiano, Adjunct Professor)

US patent 8,394,984 B2 describes a process to produce ethyl acetate with an option to coproduce ethanol. The process allows for the recovery of an ethyl acetate solvent, optionally with the recovery of ethanol, from a crude product obtained from the hydrogenation of acetic acid. Separation and purification processes of the crude product are employed to allow recovery of the ethyl acetate solvent.

There are four preliminary process diagrams that are options offered. Your team should note that patents are written to describe a process in this case; show operating conditions for reactions and in this case alternative process schemes, while not necessarily providing the details of the best solution. Overall conditions must be included, but can be somewhat disguised to safeguard confidential data. Your team's task is to decide on the most economical process that is based on the given schemes. Be certain to impose your own creativity to determine a better scheme, if possible.

Since the process can be designed to produce only ethyl acetate or to produce an ethanol coproduct, your team, "Top Guns", is asked to make the economic decision of producing only one product or both. Your management have in mind that a plant capacity of 100 million pounds per year to 200 million would be a target. You are tasked with further research into the market for these products to recommend the facility capacity based on market projections. This market research will include the search for the best supply location of the raw materials required. Your team will decide whether to build your facility near the raw material supply, the customer base locations or a central complex owned by your company in the Houston, TX area. Then all utilities and other auxiliaries will be available at current costs.

Management's focus will be on maximizing the internal rate of return based on capital employed. Environmental and safety considerations should be discussed in your final report.

Reference

US 8,394.984 B2, Process for producing an ethyl acetate solvent and co-producion of ethanol, Johnson et. al., 2013

7. Formulation of a High-Volume Small Molecule Drug Product (Recommended by Alex Marchut, Esperion)

Background

Most small molecule Active Pharmaceutical Ingredients, API's, are formulated into tablets in large batches on the order of millions of tablets or more. The Critical Quality Attributes, CQA's, are typically the assay of the API and dissolution measured in vitro as well tablet properties such as weight, thickness, hardness and appearance. A typical process to formulate the API would include some type of granulation of the API, blending of the granules with other solids, compression of the blend into tablets, and application of a coating to give the tablets the required appearance. Recently continuous manufacturing of tablets has become more and more popular in the pharmaceutical industry due to advantages inherent to continuous manufacturing for high-volume products. In both cases, batch and continuous manufacturing, modern facilities are typically built with a good deal of automation so that paper batch records are not required, and data is automatically gathered electronically.

Project Statement

You will be working on a project where you must design a process to formulate Clairatenol a blockbuster drug product with anticipated sales of 1 billion tablets per year, and design the production facility in which it will be manufactured. You should evaluate both batch and continuous manufacturing and target a cost for conversion into tablets of 1 cent per tablet. The granulation step can be run in a high shear granulator in the case of batch production or in a twin-screw granulator in the case of continuous manufacturing. The blending step can be run in a bin blender in the case of batch production and in a continuous blender in the case of continuous manufacturing. In both cases the tablet press will be the same or similar. The tablet is coated but a reliable continuous tablet coater may not be commercially available so unless one is recommended by the project team, the coating can be done in a "semi-batch" mode in the case of continuous production. Semi-batch coaters for continuous manufacturing of tablets are typically smaller coaters where the cycle time of the coating batch is matched with the throughput of the continuous line such that it is always in use (including charging and discharging).

Once you have designed the process, you will need to design the manufacturing facility, keeping in mind the differences in the size of the equipment and how that will impact the footprint of the facility. As you design the facility, you should do your best to keep capital costs of the equipment and operating costs of the facility to a minimum. You can build the plant 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 facility should be designed so that the operators are safe from hazards like inhaling dust from the powders, no waste is released to the environment, and any risks of dust explosions are accounted for in the design. The final design should compare a batch and a continuous process, ultimately making a recommendation as to which is a wiser investment.

8. CO_2 Capture and Conversion with Binding Organic Liquids (Recommended by Dr. Matthew Targett, SpruceWorks LLC)

Overview

The transformation of captured CO_2 into value-added chemicals to mitigate increasing CO_2 concentration in the atmosphere has gained significant attention recently. The capture of CO_2 from emission sources as well as from air represents a process of paramount importance in view of the increasing CO_2 concentration in the atmosphere and its associated negative consequences on the biosphere. Once captured using various technologies, CO_2 is typically desorbed and compressed for either storage (carbon capture and storage (CCS)) or production of value-added products (carbon capture and utilization (CCU)).

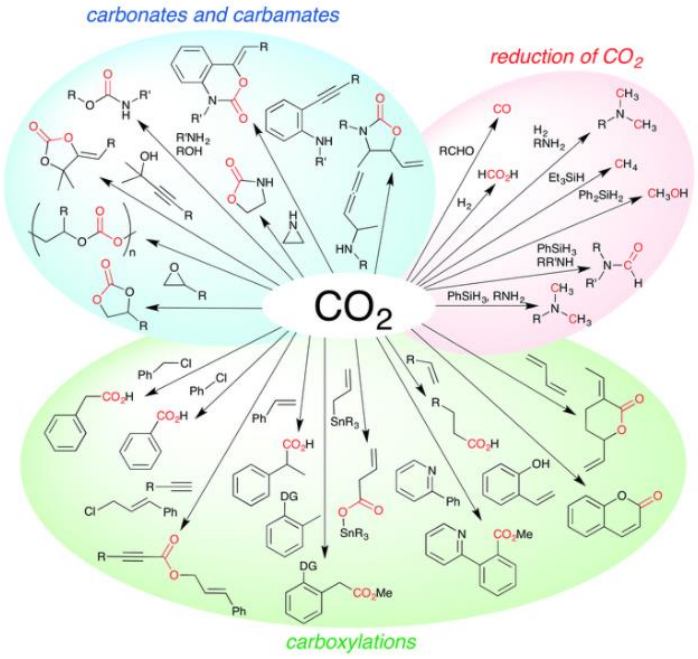

FIGURE 1: Examples of Chemical Fixation of CO_2 [1]

As shown in Figure 1, numerous products can be made from CO_2. Among various products that can be synthesized from CO_2, methanol and formic acid are of high interest because they can be used directly as fuels or to generate H_2 on demand at low temperatures (<100 °C), making them attractive hydrogen carriers. Methanol is already produced in huge quantities worldwide (100 billion liters annually) and is also a raw material for many chemicals and products, including formaldehyde, dimethyl ether, light olefins, and gasoline.

Though carbon capture and storage (CCS) is already being practiced in a few places, it suffers from energy-intensive CO_2 desorption and compression steps involved, which can be avoided in a novel integrated carbon capture and utilization (CCU) approach, especially in systems where the same solvent can be used for both capture and conversion, and condensed phase reactions could promote cost and energy advantages versus incumbent technologies.

[1] Recent Progress in Catalytic Conversions of Carbon Dioxide; Maeda etal; Catal. Sci. Technol., 2014, 4, 1482-1497

Recent CO_2 capture and conversion studies [2,3] at the US Dept of Energy's Pacific Northwest National Laboratory (PNNL) indicate that these new approaches are possible through an Integrated Capture and Conversion to Methanol (ICCM) process as shown pictorially below.

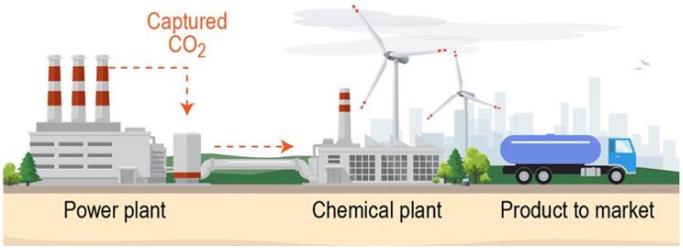

FIGURE 2: Integrated Capture and Conversion to Methanol (ICCM Process) Source: Pacific Northwest National Laboratory and SoCalGas

ICCM uses flue gas from an industrial source, cools the gas and then runs it through a CO_2 absorber. In the absorber, CO_2 is captured by PNNL's proprietary 'Carbon Dioxide Binding Organic Liquids' solvent. The solvent is then pressurized, heated and passed through to the main reactor, along with hydrogen, for methanol production. The reactor produces a methanol and water mixture which is then pumped into a distillation column designed to produce methanol at a purity of 99.6%. The excess hydrogen and solvent from the reactor are recycled back to the CO_2 absorber. A generalized process schematic of ethanol-assisted CO_2 capture and hydrogenation to produce methanol and water is shown below in Figure 3.

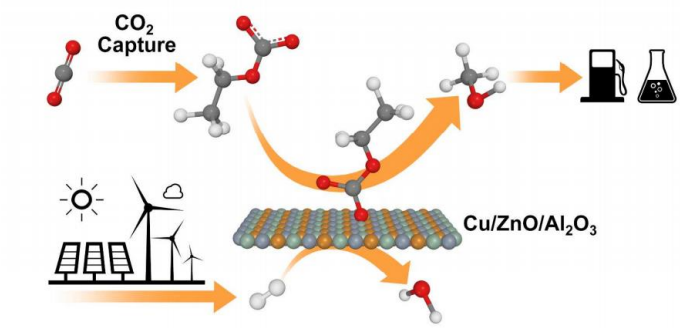

FIGURE 3: Generalized Schematic of Ethanol-assisted CO_2 Capture and Hydrogenation to produce Methanol and Water [4].

Project Statement

For the purposes of this project, the objective will be to determine the optimal commercial process configuration for capturing CO_2 and for converting CO_2 into methanol. It is recommended to base the main capture process directly upon the experimental data reported in PNNL's binding organic liquid (BOL) CO_2 capture studies [5]. And hydrogenation processing step directly upon PNNL's CO_2 conversion studies [3].

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[2] https://www.energyglobal.com/other-renewables/26112019/us-department-of-energy-to-fund-carbon-capture-project/

[3] Condensed-Phase Low Temperature Heterogeneous Hydrogenation of CO_2 to Methanol, Kothandaraman etal; Catal. Sci. Technol., 2018, 8, 5098

[4] ibid

[5] a) Organic Liquid CO_2 Capture Agents with High Gravimetric CO_2 Capacity, Heldebrant etal.; Energy Environ. Sci., 2008, 1, 487-493; b) Improving the Regeneration of CO_2-Binding Organic Liquids with a Polarity Change, Mathias etal.; Energy Environ. Sci., 2013, 6, 2233; c) Bench-Scale Testing and Process Performance Projections of CO_2 Capture by CO_2−Binding Organic Liquids (CO_2BOLs) with and without Polarity-Swing-Assisted Regeneration, Zheng etal.; Energy Fuels, 2016, 30, 1192-1203

In terms of a rigorous and detailed project structure, the following approach is recommended at the outset. The key to a techno-economic evaluation success is a sufficiently accurate process simulation model covering major processing steps; namely, adsorption, hydrogenation, purification and solvent recycle steps as shown below in Figure 4.

The main refining steps of solvent (s) recovery need to take into account integrated energy saving heat integration schemes, especially given the exothermic nature of the hydrogenation step. The process simulation model should take into account user-defined Key Input Variables (KIVs) and have the ability to predict Key Output Variables (KOVs). Some of the key input variables will be fixed.

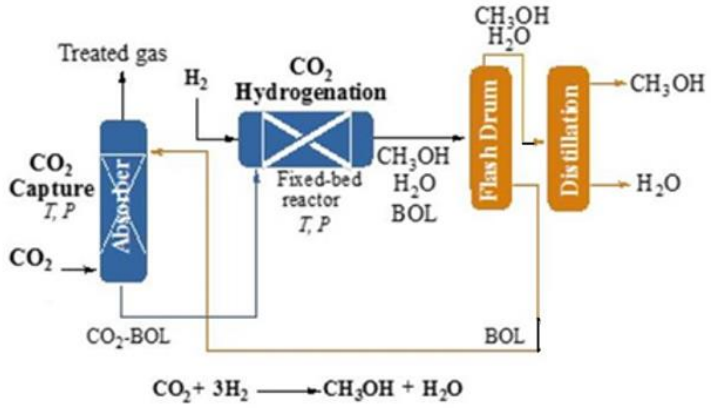


FIGURE 4: Example Process Configuration for ICCM

Project Statement – defined criteria

Overall

- Capacity: 100 TPD CO_2 feed rate
- Process Inputs: CO_2, H_2, BOL, catalyst
- BOL (recommended): NEt_3 in combination with EtOH

CO_2 Capture

- CO_2 feed composition, to be determined by other references and mass balance estimations
- T, P, res time : as indicated in cited reports
- % CO_2 capture from feed (tbd)

CO_2 Hydrogenation

- T, P, res time : as indicated in cited reports, roughly 25 bar & 120^oC
- H_2/CO_2 feed slightly higher than stoichiometric to shift reaction equilibrium and increase CO_2 conversion
- Produce methanol at a purity of 99.6%
- % CO_2 feed conversion to methanol: tbd depending costs of full conversion versus product separation and recycle

Key Input Variables – to be varied for the purposes of determining lowest Capex-Opex operation

- absorber design (temperature, volume) depending on VLE and adsorption kinetics
- heat integration design

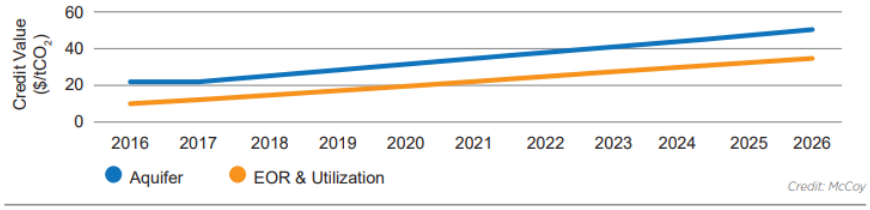
Key Output Variables – to be determined by modelling

- OPEX cost, $ per ton of liquid products
- Capex investment, $ per ton of annual CO_2 consumption
- IRR/NPV

• Financial projections must take into account tax credits for CO_2 utilization as indicated in section 45Q of US tax code.[6]

45Q, Types of Sources and Credit Between 2018-2026

	Threshold by Facility Type ($ktCO_2/y0$)			Credit in 2026 ($/t)
	Power Plant	Industrial Facility	Direct Air Capture	
Dedicated Storage	500	100	100	50
EOR	500	100	100	35
Utilization	25	25	25	35



[1] *$35/ton for EOR and $50/ton for saline storage, available indefinitely*

Note: The author of this project is not based in Philadelphia. Many or all interactions will be through Zoom, phone and/or email.

[6] https://www.energy.gov/sites/prod/files/2019/10/f67/Internal%20Revenue%20Code%20Tax%20Fact%20Sheet.pdf

9. Clean Energy with CO_2 Sequestration by Allam Cycle (Recommended by Adam Brostow, Honeywell-UOP)

Preventing global warming by keeping temperature rise below 1.5 deg. C is one of the most critical issues facing humanity today. Droughts, floods, hurricanes are increasing in intensity.

Your mission, should you choose to accept it, is to design two 300-MW power plants, one using the Allam cycle with CO_2 sequestration, the other one using a conventional combined cycle, and compare the two. The site conditions are as in the referenced paper on the Allam cycle (ambient conditions, cooling water, etc.).

The design team will simulate both options and compare the Allam cycle to the next best alternative (NBA). The first step would be to simulate the natural gas-fired combined cycle (NGCC). The next step would be to simulate the Allam cycle. Some unit operations can be treated, at least initially, as black boxes, with the answer refined depending on the project's progress. The authors of the Allam Cycle article have an interesting idea but are not cryogenic air separation unit (ASU) experts and may have missed something. The problem author has designed three working ASUs (Texas, Canada, India) and has direct experience with gas turbines and steam turbines and can provide detailed guidance. The students should calculate or estimate capital expenditure (CAPEX) and the operating cost (OPEX).

Some questions that remain to be answered are: can we sequester CO_2 from the combined cycle? Can we produce liquid CO_2 instead of pipeline gas as the product of the Allam cycle? How much incremental cost is involved? How would the economics look like for a 1000-MW plant?

Fig. 1

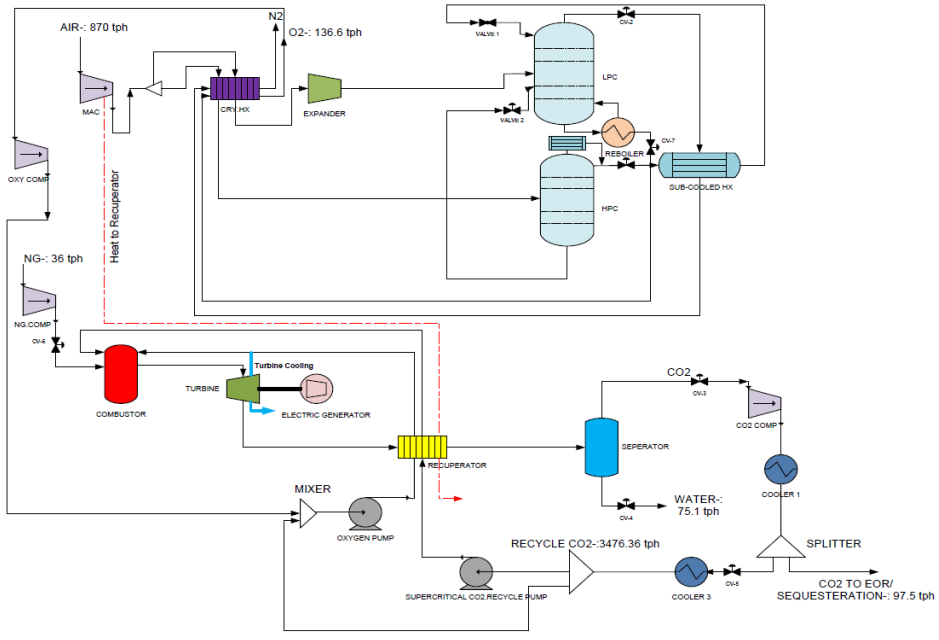


Fig. 1 shows the Allam power generation cycle with CO_2 sequestration.

Fig. 2

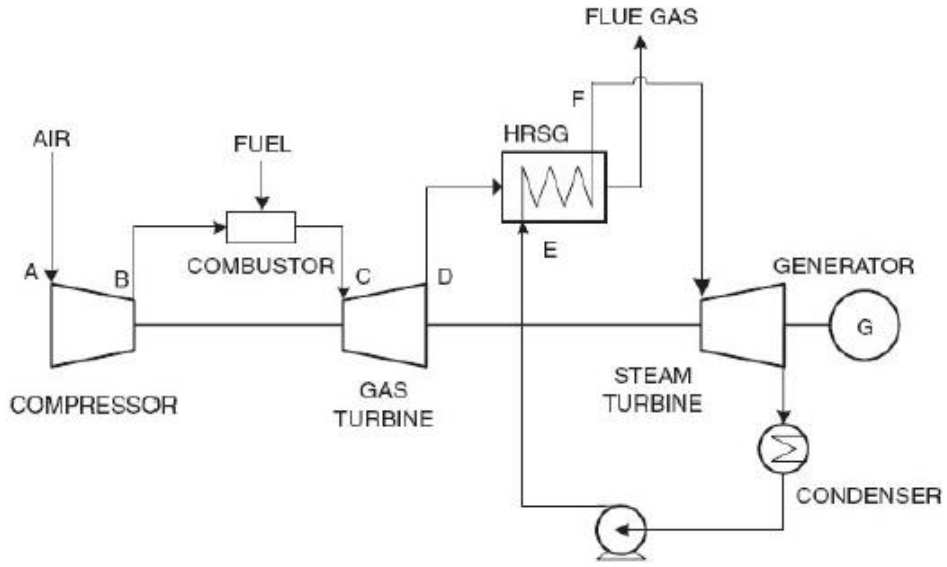


Fig. 2 shows the NBA (next best alternative), the combined cycle.

References

Allam Cycle link:
https://en.wikipedia.org/wiki/Allam_power_cycle

Combined cycle:
https://en.wikipedia.org/wiki/Combined_cycle_power_plant

Process and Carbon Footprint Analyses of the Allam Cycle Power Plant Integrated with an Air Separation Unit, Fernandes et. al., Clean Technol. 2019, 1, 325–340.

Life Cycle Assessment of a Natural Gas Combined-Cycle Power Generation System, Spath et al:
https://www.nrel.gov/docs/fy00osti/27715.pdf

Rules of Thumb for Chemical Engineers by Branan

Become an Inventor by Adam Brostow (on Amazon):
https://smile.amazon.com/Become-Inventor-Idea-Generating-Problem-Solving-Techniques/dp/1508936838/

Note: The author of this project is not based in Philadelphia. Many or all interactions will be through Zoom, phone and/or email.