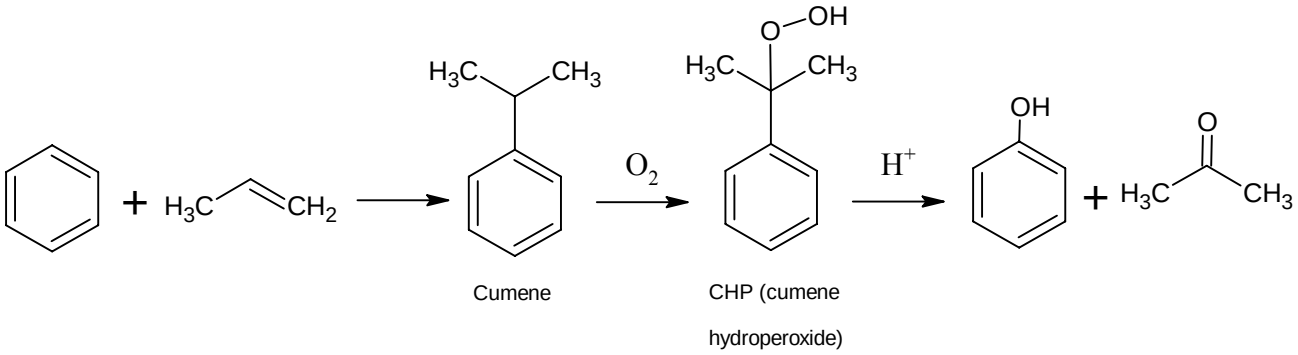
Suggested Design Projects – 2010-2011

1. Direct Route to Phenol From Benzene (recommended by Bruce M. Vrana, DuPont)

Phenol is a major chemical intermediate used in a variety of other products. Phenolic resins are used in a wide range of products, including printed circuit boards. Phenol is a raw material to make polycarbonate, used in CD and DVD discs. Phenol can be converted to caprolactam and ultimately nylon-6, or to adipic acid and ultimately nylon-6,6, used for fibers and engineering polymers. There are a wide variety of other applications for this versatile intermediate.

Phenol is conventionally made from cumene using the following chemistry:



Cumene CHP (cumene hydroperoxide)

This route has several drawbacks. Growth in demand for propylene has exceeded the growth in supply, driving propylene prices higher. Also, one mole of acetone is made per mole of phenol. The acetone must be sold at a reasonable price in order to have favorable economics on making the phenol. Although acetone has numerous uses, phenol producers often have difficulty selling the byproduct at an attractive price. Effectively, this process converts high value propylene into low value acetone. In fact, although you could sell more phenol, your company has decided to not expand phenol capacity if it produces acetone as a coproduct.

A team of chemists at the Council of Scientific and Industrial Research (CSIR) in New Delhi has recently patented a direct process from benzene to phenol, using hydrogen peroxide, a chemical which your company also makes in large quantity. While other companies have patented similar chemistry, they have all been plagued by yield loss to over-oxidized byproducts which have no end use. The team in India has measured 53% benzene conversion and 100% selectivity to phenol.

Your company is considering licensing this technology. Your team has been assembled to determine whether the process will be economical before engaging in any discussions with CSIR. Because these negotiations can be sensitive, your management has forbidden any form of contact with anyone at CSIR during your design. You may use only information

that you can find in the public domain, in the patent, on the Internet, etc. The objective is to obtain a license at the lowest possible price, so you do not want to tip off your company's interest in the process until your engineering analysis is complete.

Design a process to make 500MM lb/yr of phenol from benzene at your plant complex on the U.S. Gulf Coast. Benzene is available on site for $0.40/lb. Hydrogen peroxide is also available on your site for $0.30/lb. Phenol is worth $0.80/lb to your company. All prices are forecasts by your marketing organization for long term average prices, expressed in 2011 dollars.

You will have to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before approaching CSIR to discuss a license. Test your economics to reasonable ranges of your assumptions. If there are any possible "show-stoppers" (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding.

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. Remember that, if the negotiations are successful, you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference

U. S. Patent 7,586,014, September 8, 2009, assigned to Council of Scientific and Industrial Research

2. Glycerol to Renewable Propylene Glycol (recommended by Bruce M. Vrana, DuPont)

Propylene glycol (PG), is used to make unsaturated polyester resins, cosmetics, aircraft deicer, environmentally-friendly (and pet-friendly) automotive antifreezes, etc. PG is conventionally made from propylene. Propylene is itself a byproduct of ethylene manufacture. Since demand for polypropylene is growing faster than ethylene, propylene is in short supply and prices are rising. Demand and prices for PG are expected to increase. And there will likely be a price premium and plenty of demand for PG made from renewable resources.

Glycerol is a byproduct of biodiesel manufacture, with relatively few industrial uses. As the production of biodiesel increases, particularly in Europe due to government regulations but also in the U.S. due to public demand for renewable fuels, the price of glycerol is expected to continue to decrease.

BASF has patented a catalyst to convert glycerol to propylene glycol in very high yield – up to 100% glycerol conversion and 98.5% selectivity. The patent does not disclose quantitatively what the byproducts are, but you can assume the 1.5% of glycerol that does not form propylene glycol goes to equal amounts of n-propanol and isopropanol.

$$CH_2OH\text{-}CH_2OH\text{-}CH_2OH + H_2 \rightarrow CH_2OH\text{-}CH_2OH\text{-}CH_3 + H_2O$$

Crude glycerol from biodiesel manufacture contains 15% water, 4% NaCl, 1% methanol. It also contains trace amounts of organic sulfur and chlorine compounds, which must be removed, as described in the patent.

Design a process to make 100MM lb/yr of propylene glycol from crude glycerol. Your plant is on the U.S. Gulf Coast. Crude glycerol delivered to you costs $0.22/lb (for the crude stream at 80% concentration). Hydrogen is available on your plant site for $0.50/lb. Renewable propylene glycol can be sold for $1.00/lb. Byproduct renewable n-propanol and isopropanol can be sold for $0.80/lb. All products will need to meet normal specs for that product. All prices are forecasts by your marketing organization for long-term average prices, expressed in 2011 dollars on the Gulf Coast.

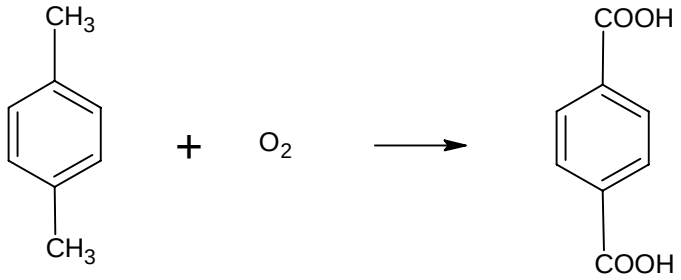
The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate. Remember that you will be there for the plant start-up and will have to live with whatever design decisions you have made.

Reference

U.S. Patent 7.790,937, September 7, 2010, assigned to BASF

3. New Terephthalic Acid Process using Ionic Liquids (recommended by Bruce M. Vrana, DuPont)

The conventional route to terephthalic acid (TPA), one of the monomers for polyethylene terephthalate (PET), is over 50 years old and has not changed much since it was discovered by Scientific Design. PET is used in soda bottles, carpets, fibers, etc. Despite the huge growth in PET worldwide, essentially all TPA is produced by the Amoco process (now owned by BP) or similar processes. In the Amoco process, p-xylene (PX) is oxidized with air to TPA, in an acetic acid solvent. Capital costs are very high because of an extremely corrosive bromide catalyst promoter, which necessitates Hastelloy or other expensive alloys be used for the equipment.



SABIC has patented a novel catalyst system which is expected to solve the corrosion problem. They use an ionic liquid with an organic cation and bromide anion (1-ethyl-3-methylimidazolium bromide). PX conversion is 100%, selectivity to TPA is 95.6%, with similar byproducts formed as the Amoco process (p-toluic acid, 4-carboxybenzaldehyde, and 4-CBA).

4-CBA is a troublesome impurity in making purified terephthalic acid (PTA). Crude TPA made by this process must be purified by dissolving the product in water and reacting the 4-CBA away, as it is extremely difficult to separate from TPA. Crude TPA has 100 ppm of other impurities, but up to 2% 4-CBA.

Your company has asked your group to assess the technoeconomic feasibility of this ionic liquid discovery. You need to design a TPA plant through production of crude TPA using this new process. Purification to PTA is outside the scope of your effort.

Obviously, corrosion is a key uncertainty of the new route. Your company's chemists believe that the ionic liquid completely prevents bromide from leaching out and corroding the equipment. Analytical results confirm that belief, but long-term corrosion tests are currently being conducted in your labs. Management wants to proceed with your study in parallel with corrosion tests. Assuming the chemists' assertion is correct, you can use stainless steel for the process. Clearly, if that is not the case, then the process would have no advantage over the Amoco process and could not afford the expensive ionic liquid promoter.

Design a process to make 800MM lb/yr of TPA from PX at your plant complex on the U.S. Gulf Coast. PX is available on site for $0.45/lb. Crude TPA is worth $0.60/lb to your company. The ionic liquid promoter is estimated to cost $25/lb when produced at the scale required to initially charge to your plant. All prices are forecasts by your marketing organization for long term average prices, expressed in 2011 at your plant site.

You will have to make many assumptions to complete your design, since the data you have is far from complete. State them explicitly in your report, so that management may understand the uncertainty in your design and economic projections before considering the next step toward commercialization – designing and running a pilot plant. Test your economics to reasonable ranges of your assumptions. If there are any possible "show-stoppers" (i.e., possible fatal flaws, if one assumption is incorrect that would make the design either technically infeasible or uneconomical), these need to be clearly communicated and understood before proceeding. Corrosion is one such show-stopper, but the question is whether there are any others.

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. Remember that, if the plant is built, you will be there for the start-up and will have to live with whatever design decisions you have made.

Reference

European Patent 2,125,686, December 2, 2009, assigned to SABIC (equivalent to World Patent application 2008/074497, June 26, 2008)

4. Algae to Biodiesel
(recommended by Warren D. Seider, UPenn, Kimberly Ogden, UArizona)

During the Spring 2010, a design project [1] focused on the growth of algae using the SIMGAE cultivation process [2-4], (2) OriginOil's process for lipid extraction [9-11], and (3) a process to convert the lipids to alkanes (green diesel) [15-16]. A profitable overall process was designed, although the investment costs were very high. Since then, a research project to convert algae to biofuels by the National Alliance for Advanced Biofuels and Bioproducts (NAABB) was funded by DOE ($49 million). The Univ. Arizona and Penn are collaborating on a portion of this project. Furthermore, some of the major oil companies (e.g., ExxonMobil) have announced significant development efforts. The advantages of algae are numerous: (1) its cultivation does not encroach on the food sector, (2) its biomass productivity per acre far exceeds that of any agricultural commodity, (3) it produces lipids that can be converted easily to biodiesel or fuel-range hydrocarbons.

In this design project, the focus will be on exploring the processing technologies described below, and likely other promising technologies that are proposed in the next few months.

Algae Cultivation

Recently, the *heteroboost* photosynthesis-fermentation process was proposed to generate lipids for biodiesel production [5]. First, *chlorella prototecoides* algae are grown autotrophically to fix CO_2. Then these are metabolized heterotrophically using glucose to significantly increase the lipid yield.

Yet, another cultivation process was recently proposed by Teymour and coauthors [6] involving a farm of artificial algae trees whose trunk and branches are filled with algae solution and exposed to solar energy.

More recently, a kinetic model has been proposed to estimate the rate of algae growth as a function of the light intensity and the concentration of nitrogen nutrients [7]. This model can be used to better estimate the size and cost of various conversion processes, including photobioreactors. Also, data taken in "raceways" at the Univ. of Arizona are showing the impact of temperature on the algae growth rate [8].

Based upon the data in [5-8], better estimates of the installation and operating costs of cultivation processes, as compared with SIMGAE process costs, should be obtained. It is anticipated that lower-cost processes will be designed.

Lipid Extraction

The OriginOil process involves the generation of sonic waves and microbubbles at high frequency [9-11]. Energy costs are claimed to be 10% of conventional processing costs. An objective of this design project will be to gain better estimates of these costs – although this aspect of the design is likely to be deemphasized.

Lipid to Biodiesel

The conversion of the lipid fraction to useful products has several options [12-14]. One approach is to convert it to biodiesel [15-16]. Recently, two papers discuss the ASPEN PLUS simulation of a potential process to produce biodiesel [17-18]. Your group will seek to improve upon these designs and will attempt to carry out design optimization. This will include sizing and costing the trans-esterification reactor and the remainder of the processing equipment.

Life-Cycle Analysis

When estimating the profitability of your entire process to convert algae to biodiesel, your group will carry out a life-cycle analysis (LCA) [19]. To achieve a sustainable design, it is important that no net CO_2 be produced, that waste water be recycled, and the like. You will attempt to optimize the profitability of your design, as well as its sustainability.

References

Algae Cultivation

1) Carlson, L.S., Lee, M.Y., Oje, C.A.E., and A. Xu, *Algae to Alkanes*, SEAS Library, Univ. of Pennsylvania, 2010.

2) Hassania, J. (Diversified Energy) "Simgae – Low Cost, Broad Application – Algal Biomass Production System" , NETL 2008 Conference Proceedings, Sept. 18, 2008 (Presentation on Simgae technology with economics) at www.netl.doe.gov/publications/proceedings/08/.../index.html

3) Editor, "Simgae – Low Cost Algae Prod. Sys.", Aug, 2007, http//www.eneverve.com (contains optimistic claims for project economics)

4) Cloud, G. et al., US2008/0311649 A1, "Pressurized Flexible Tubing System for Producing Algae", Dec 18, 2008, XL Renewables

5) Xiong, W., Gao, C., Yan, D., Wu, C., and Q. Wu, "Bouble CO2 Fixation in Photosynthesis-Fermentation Model Enhances Algal Lipid Synthesis for Biodiesel Production, *Bioresource Tech.*, **101**, 2287-2293 (2010).

6) Eltayeb, A.E., Khalil, O., Al-Hallaj, S., and F. Teymour, "Design and Modeling of Optical Modules for Use in the Emerald Forest Algae Photobioreactors," *Comput. Chem. Eng.*, **34** 1323-1340 (2010).

7) Packer, A., Li, Y. Andersen, T., Hu, Q., Kuang, Y., and M. Sommerfeld, " Growth and Neutral Lipid Synthesis in Green Microalgae: A Mathematical Model," *Bioresource Tech.*, in print.

8) Waller, P., "Raceway Developments and Temperature Effects for Arid Climates,"

POWER POINT presentation, July 2010.

Lipid Isolation

9) Chementator News Item, "A One-Step Process for Extracting Oil from Algae", *Chem. Eng.*, June 2009

10) Eckelberry, N. and T.R, "Algae Growth System for Oil Production", US2009/0029445 A1, Jan. 29, 2009 (describes OriginOil's first-generation extraction technology)

11) OriginOil.com – Website contains video of lipid extraction process

Lipid Processing

12) Huber, G.W., O'Connor, P., and A. Corma, "Processing Biomass in Conventional Oil Refineries," *Applied Catalysis A*, **329**, 120-129 (2007).

13) Stiefel, S., and G. Dassori, "Simulation of Biodiesel Production through Transesterification of Vegetable Oils," *Ind. Eng. Chem. Res.*, **48**, 1068-1071 (2009).

14) Moser, B.R., "Biodiesel Production, Properties, and Feedstocks," *In Vitro Cell Dev. Biol.*, **45**, 229-266 (2009).

15) Machacek, M. T. et al., "Continuous Algal Biodiesel Production Facility", US2009/0071064 A1, March 19, 2009 (describes ASPEN PLUS Simulation of lipids to biodiesel)

16) Doviak , S., Long, M., Peck, S., and J. Yuen, *Green Diesel Fuel: A Biofuel Process*, SEAS Library, Univ. of Pennsylvania, 2008.

17) Chung, A.-F., and Y.A. Lui, "Integrated Process Modeling and Product Design of Biodiesel Manufacturing," *Ind. Eng. Chem. Res.*, **49**, 1197-1213 (2010).

18) Pokoo-Aikins, G., Nadim, A., El-Halwagi, M.M., and V. Mahalec, "Design and Analysis of Biodiesel Production from Algae Grown Through Carbon Sequestration," *Clean Techn. Environ. Policy*, **12**, 239-254 (2010).

LCA

19) Aresta, M. et al., "Utilization of macro-algae for enhanced CO_2 fixation and biofuels production: Development of a computing software for an LCA Study, "*Fuel Processing Technology*" 86 (2005), 1679-1693.

5. Propylene from Biomass
(recommended by John A. Wismer, Arkema)

The conversion of biomass to petrochemicals has been a subject of active research for over 40 years. The economics of breaking down biomass to its primary molecular building blocks – known as a synthesis gas – then building the synthesis gas back up to petrochemicals have always proved inferior to that of fossil fuel-based processes. Recent shifts in feedstock prices and technology improvements indicate that this may be changing. Haldor Topsoe recently announced plans for a large-scale process to make DME from wood chips. Separately, JGC has announced a DME-to-propylene pilot plant. Your client is a large multinational oil company that has taken notice of these developments. They want to know whether or not propylene can be economically made from a biomass feedstock using an integration of best available technology. A processing rate of 1.5 million metric tons of dry biomass/yr is the baseline capacity.

Propylene has traditionally been produced as a co-product in steam crackers or as a refinery by-product. Recent disproportionate demand increases have forced the petrochemical industry to explore on-purpose production. This type of processing – either propane dehydrogenation or ethylene metahesis – currently accounts for about 5% of total production. Alternative supply chains are currently being pursued by a number of companies. One potential source is methane. Another possible source is cellulosic biomass – a precursor that yields a synthesis gas that is superior in composition than methane-derived gas with respect to conversion to basic petrochemicals.

Wood chips or sawdust can be converted into synthesis gas (or syngas) gas by pyrolysis. Since the original wood contains C, H, and O, the resulting synthesis gas has a composition of CO, CO_2, H_2, and H_2O that reflects the elemental ratios in the original wood. The CO_2 is normally considered to be undesirable. However, if the syngas is to be converted to dimethyl ether (DME), the CO_2 has the net effect of shifting the equilibrium towards DME. Furthermore the syngas produced from biomass has a higher CO/H_2 mol ratio than that produced from steam reforming of methane. The pyrolysis is very endothermic. Heat integration with the rest of the process is a must.

The biomass syngas can be converted to DME or a mixture of DME and methanol in a catalyzed reactor. The main reactions are:

$$1)\ CO + 2H_2 \leftrightarrow CH_3OH$$

$$2)\ CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$$

$$3)\ 2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$$

$$4)\ CO + H_2O \leftrightarrow CO_2 + H_2$$

All of these reactions are reversible. Also, they are all exothermic to varying degrees so that higher temperatures tends to decrease DME formation. Reference 4 illustrates a

number of different reactor configurations, all of which operate in a mixed phase and have moderate productivities. Reference 8 shows a crude material balance and conceptual flowsheet for DME production starting from biomass. Reference 6 claims that the reactor productivity (i.e., conversion per pass of CO and DME selectivity) can be dramatically improved through the use of a micro-channel reactor configuration. A previous senior design project[14] used micro-channel reactors and can be used as a design guide.

The net reaction for the DME to propylene reaction is:

$$5)\quad 3CH_3OCH_3 \quad \rightarrow \quad 2CH_2{=}CHCH_3 + H_2O$$

The reaction is mildly exothermic. It should be noted that most patents cite a mixture of methanol and DME as a feedstock. The advantage of maximizing the DME/methanol ratio is that it reduces the overall heat of reaction. One design decision is whether to separate and recycle the methanol to the DME reactor or send it forward to the olefin reactor. Reference 12 claims an overall yield of 70%. The literature suggests that the best single pass yield is about 45%. However, the patent in Reference 11 suggests that heavier olefins and alkanes can be recycled to the reactor giving a reasonable conversion to propylene. At any rate, you should manipulate the material balance to achieve the 70% overall propylene yield. Everything else gets disposed of at fuel value.

References

Wood to Syngas

1) Dufour, A., et al., "Synthesis gas production by biomass pyrolysis: Effect of reactor temperature on product distribution", Int'l. J. Hydrogen Energy **24** (2009), 1726-1734.

2) Pengemi, L., et al., "Bio-syngas production from biomass catalytic gasification," Energy Conv. and Management, **48** (2007) 1,132-1,139.

3) Baratieri, et al., "The use of biomass syngas in IC engines and CCGT plants: A comparative analysis", Appl. Thermal Eng., **29** (2009), 3,309-3,318. (note flowsheet).

Syngas to DME

4) U.S. Patent 6,191,175 B1 (2001). Assigned to Haldor-Topsoe, "Process for the Synthesis of a Methanol/Dimethylether Mixture from Synthesis Gas."
.

5) Wang, L., "Influence of reaction conditions on methanol synthesis and WGF reaction in the syngas-to-DME Process," J. Natural Gas Chem., **15** (2006), 38-44.

6) Hu, J., et al., "Conversion of biomass syngas to DME using a micro-channel reactor," Ind. Eng. Chem. Res., **44** (2005), 1,722-1,727.

7) Larson, E., et al., "Large-scale gasification-based coproduction of fuels from electricity

and switchgrass", Biofuels, Bioproducts, and Biorefining, **3**(2) (2009), 174-194. (Note conceptual flowsheet includes CO_2 removal).

8) Consonni, S., et al., "A gasification-based biorefinery for the pulp and paper industry (Note the conceptual flowsheet with crude material balance.)

DME to Propylene

9) Zhao, T.-S., et al., "Direct synthesis of propylene and light olefins from dimethylether catalyzed by modifeied H-ZSM-5", Catalysis Comm., **7** (2006), 647-650.

10) U.S. Patent 2003/014319 (Inomata, et al.), "Process for the Preparation of Lower Olefins"

11) U.S. Patent 5,981,819 (Assigned to Metallgesellschaft Aktiengesellschaft), "Process of generating C_3 and C_4 olefins from a feed Mixture containing C_4 and C_7 olefins.

Miscellaneous

12) "Demonstration for wood-to-fuel via DME Route", Chem. Eng., Jan. 2010, p. 16

13) "DME to Propylene", Chem. Eng., Jan. 2010, p. 14.

14) Hammond, J., et al., "Alaskan natural gas to liquids (GTL) using micro-channel reactors" 4-14-09, Penn – CBE 459 Design Project

6. Renewable 1,4-Butanediol (recommended by Stephen M. Tieri, DuPont)

1,4-Butanediol (BDO) is a critical raw material for the production of polymers used to make spandex, automotive plastics, and performance thermoplastic elastomers. The majority of the world BDO production goes into tetrahydrofuran (THF) (an intermediate for spandex and other performance polymer production) and polybutylene terephthalate (PBT) for engineering plastics. There are several traditional petrochemical routes to BDO, including the Reppe, Propylene oxide, Davy, Mitsubishi, and Geminox processes. As a result of climate change, dwindling petroleum resources, and desire for energy independence; there has been significant research and investment in the last decade to develop technologies which reduce energy consumption, improve efficiency, and produce materials and fuels from renewable resources. Government grants and subsidies as well as consumer demand are driving the intense industrial and academic competition to develop bio-based and sustainable materials; with equivalent functionality to the traditional petrochemical derived materials, but derived from renewable sources and with reduced environmental burden.

Through its research efforts, your company has developed new and innovative technology to produce 'green' BDO, through conversion of biomass-derived and renewable feedstocks, rather than crude oil or natural gas. Specifically, the research group developed a direct, bio-based production route with fewer steps than the traditional petrochemical processes. As the 1,4-butanediol from this technology has the identical structure and functionality of traditional 1,4-BDO, it serves as a direct replacement for petroleum-based BDO, to produce renewably-sourced polymers without modifications to downstream equipment or processes.

The microorganism and process have been tested across a variety of commercial feedstocks, with no apparent loss in key fermentation performance metrics or final product quality. Successful pilot trials this summer produced material from a 3,000 gallon fermentor and purified it to greater than 99%, reaching over 80 gm/liter titers in fermentations. Results from pilot-plant operation indicated that product yield, microbiological productivity, separation, and purification were on-target to deliver cost advantages at commercial scale. Now that the research, development, and pilot teams have succeeded in achieving their milestone targets, corporate leadership is confident to proceed to the first commercial-scale production facility.

Your project team has been assembled to design the commercial demonstration plant for this new sustainable technology. The business objective is to design a commercial scale facility to produce 50 MM lb/yr of 1,4-butanediol from a renewable sugar feedstock. The BDO product purity and quality will need to meet or exceed current commercial requirements for polymer-grade material, to be acceptable to perspective customers.

For this project, your company negotiated an agreement with a world leader in agricultural processing to supply sugar feed to the plant and process. The renewable BDO plant will be co-located on a site with one of the partner's existing facilities. Based on your input, the

partner will expand either one of its ethanol dry mills in the Midwestern United States, or one of its sugar and ethanol facilities in Brazil to provide sufficient sugar capacity to meet the BDO process requirements. Sugar supply from the dry mill is expected to be typical of that currently used to supply fuel ethanol fermentations, while the Brazilian facility will supply molasses and cane juice at standard cane industry concentrations. In addition to raw material economics, your team will need to carefully consider the advantages, disadvantages, potential obstacles, and restrictions for each sugar supply option when making its selection. (Example: The sugar-cane crushing season in Brazil is 8-9 months long.) Current market pricing is to be expected for all raw materials, utilities, and product, regardless of location.

The company intends to use this technology to attract additional investors, industrial partners for both feedstock supply and sustainably branded polymers. Although your company expects to build and operate this commercial facility, in addition to some future sister facilities, current corporate business strategy also plans to license the technology as an additional revenue source. To this end, your corporate marketing group plans to advertize this technology on the basis that the process and product costs less to build and manufacture, compared to conventionally-produced BDO. Therefore, as a part of your financial analysis, your team will need to determine an appropriate technology licensing fee.

The plant design should be as environmentally-friendly as possible, and as required by state and federal emissions legislation. 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. As the process technology 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 that given here and listed in the references below. Cite any literature data used. If required, make reasonable assumptions, state them, and state whether your design or economics are sensitive to the assumptions you have made.

References

- 20100112654 Microorganisms for the Production of 1,4-Butanediol (U.S. Patent Application)
- 20090075351 Compositions and Methods for the Biosynthesis of 1,4-Butanediol and its Precursors (U.S. Patent Application)
- 20090047719 Methods and Organisms for the Growth-coupled Production of 1,4-butanediol (U.S. Patent Application)
- http://www.genomatica.com
- http://www.genomatica.com/pdf/SpecialtyChemicals.pdf
- http://www.genomatica.com/archives/1581
- The Renewable Fuels Association web site has a good description of the fuel ethanol process and industry. http://www.ethanolrfa.org

- A good model for much of the dry grind ethanol process is discussed on http://www.intelligen.com/literature.shtml which links to a paper by Kwiatkowski et al. This includes a SUPERPRO DESIGNER model that works with their evaluation version of the software. Note, however, that SUPERPRO DESIGNER does not handle VLE rigorously and thus is not suitable for designing this process.
- Web resource for sugar & sugar solution properties (including molasses), with references for items common to the sugar and ethanol industries. http://www.sugartech.co.za/matlprop/index.php
- www.ams.usda.gov

7. Renewable Bio-Monomer Pilot Plant (recommended by Stephen M. Tieri, DuPont)

Global climate change, dwindling petroleum resources, and a desire for energy independence, have driven significant research and investment in the last decade to develop technologies that reduce energy consumption, improve efficiency, and produce materials and fuels from renewable resources. Industry stakeholders, including corporate executives, employees, and customers, are now insisting on the development and incorporation of sustainably produced materials, in place of traditional petroleum sourced chemicals and derivatives. Recent increases in oil prices are assisting in the growing economic viability and commercial potential for conversion of renewable raw materials to basic chemicals and functional intermediates. Biomass derived sugars provide opportunities for new, and potentially low cost, routes to chemical intermediates. However, the disposition of agricultural resources and production to support both this transition from petroleum to renewable fuels and provide food to meet the demands of the increasing global population is a continuing source of controversy and significant discussion.

Your company, through its research efforts, has developed new and novel bio-based, bio-catalyzed, routes to commercially important intermediates and basic chemicals. Among the most promising new technologies developed at laboratory scale are routes to the methacrylic acid and methylethylketone (MEK). Your company strongly believes bio-based sugars will provide a price stable feedstock alternative, and will positively contribute to the overall process environmental life-cycle analysis. In addition to being cost competitive with conventional processes-derived materials, the bio-derived monomers must provide the same level of purity and reactivity for producing polymers, downstream intermediates, and polymeric derivatives. Based on initial laboratory results and testing, company leadership has confidence that the new bio-process will be economically competitive and attractive, with the additional development work that naturally comes with standard technology commercialization programs. Business leadership is eager to proceed with the next phase in commercializing these technologies, and has agreed to fund a new facility to conduct pilot testing for these products and processes.

Your team's objective is to design the pilot facility to demonstrate the operation of the technology and develop critical process data for commercial design to produce methacrylic acid and MEK from cane sugar supplies. The primary function of this pilot plant is to generate data applicable to potential commercial scale processes, in current corporate business forecasts for Brazil. While considerable development resources have been spent on the biocatalyst (microorganism), less work has been completed with respect to the subsequent separation and purification of the individual materials. Therefore, your team will need to identify the most commercially viable separation technologies to include in the process design for each individual material. Each product will need to be separated from the fermentation broth and purified to meet or exceed standard commercial concentrations and quality measurements for polymer grade material.

The facility is expected to provide equal quantities of each material for market demonstration testing, initial customer qualification testing, as well as produce representative waste material for treatment approval and potential agronomic acceptance (if a stream similar to the Vinasse from a sugar cane ethanol production mill is identified). Although the goal for pilot operation is data generation, a minimum of 30 M kg/yr of each individual monomer product (60 M kg/yr total) is expected to be necessary to complete the market demonstration and qualification testing. As the facility is expected to explore the bounds of the process technologies, the business is willing to accept reasonable uptimes for this type of work in the first two years of pilot operation. While operation of the processes at the pilot scale is not expected to hit all economic targets for commercial viability, it is necessary to provide corporate leadership with an estimate of the overall pilot program costs, for an expected 5-year pilot development program. Monomer product within commercial specifications can be sold at current market pricing, without restriction, to help defray the pilot operational costs, as raw materials and utilities will be charged at current market pricing. It is also expected that successful pilot trials will support validation of commercial scale economic estimates.

Corporate leadership has identified a partner willing to host the proposed pilot plant, and supply sufficient molasses, cane juice, and utilities to support the development testing. The pilot facility will be located on the site of a current sugar and ethanol facility in the Sao Paolo region of Brazil. While the pilot plant will not require separate raw material storage facilities and utilities, the design will need to include the equipment reasonably necessary to transfer materials from the main plant's current storage and supply facilities. Based on the standard cane crushing season, it is expected that you will have access to a sugar supply from the plant's main storage tanks for 9 months/yr.

The pilot-plant equipment should allow for flexibility to investigate a wide range of operating conditions and to identify optimal process conditions for use in the future commercial facility, for each individual product.
Process parameters which are expected to be explored during the course of pilot trials include, but are not limited to, sugar feed concentration (molasses only, cane juice, or mixture), fermentation productivity, and separation process configuration.

The pilot facility is not expected to be a "showplace" facility, where external people are routinely given tours and used as a "sales device", but one where the technology and full process are demonstrated, studied, and optimized to produce a robust technology package for future commercialization. While corporate and business leadership understand that this facility is expected to handle the development work for several new technologies, explore optimal ranges of multiple processes, and handle hazardous materials, the budget is not unlimited, and there is an expectation that most (if not all) equipment will be shared between both products. However, due to the hazards present inherently with some of the products, it is critical that the pilot equipment safely handle all of the intended products and any isolated intermediates.

The pilot-plant design should be as environmentally-friendly as possible, and as required by state and federal emissions legislation. Recover and recycle process materials to the

maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The pilot-plant design must also be controllable and safe to operate. As the process technology 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 that given here and listed in the references below. Cite any literature data used. If required, make reasonable assumptions, state them, and state whether your design or economics are sensitive to the assumptions you have made.

References

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- 20080199926 Methods and Organisms for Growth-Coupled Production of 3-Hydroxypropionic Acid
- 20070111294 Methods and Organisms for the Growth-Coupled Production of Succinate
- http://www.genomatica.com
  Web resource for sugar & sugar solution properties (including molasses), with references for items common to the sugar and ethanol industries.
  http://www.sugartech.co.za/matlprop/index.php

8. Membranes for Olefin Separations (recommended by Gary A. Sawyer, Lyondell)

Your company is a major producer of membranes used in water purification, natural gas purification, and carbon dioxide removal. Your R&D department has developed membranes for a new market application, that of olefin/paraffin separation. You have been charged with doing a market penetration feasibility study. The market of primary interest is in propylene/propane separation, which is typically done with conventional distillation.

Polymer grade propylene (99.5 wt% propylene) is nearly a 70 million metric ton per year global business, and is expected to grow at 5%/yr. To meet demand, new capacity will be based on steam cracker technology or propane dehydrogenation technology, both of which separate propylene from a mixture of propylene and propane in a distillation operation known as a "C3 Splitter". The steam cracker feed to the C3 splitter could also be sold as "chemical grade propylene". The table below shows typical feed rates and compositions for the C3 splitter in a world-scale plant of each technology.

Table 1

C3 Splitter Sizing Basis	Product Rate, thousand Metric Tons/yr	Feed Wt% Propylene / Propane	Feed Condition
Steam Cracker	600	93% / 7%	80ºF, 275 psig
Propane Dehydrogenation	500	35% / 65%	150ºF, 450 psig

Membranes

Separation of hydrocarbon gases using membrane technology represents an attractive energy-saving opportunity for modern petrochemical facilities. Membrane technology can be more energy efficient for difficult separations than distillation columns requiring high internal reflux. Traditional membranes operate on a principle of size selectivity and allow smaller molecules to permeate through the membrane leaving larger molecules behind. In engineering terms, membranes operate on the principle that the flux rate (mass flow rate per unit area) across the membrane of individual chemical species in a mixture depends on the type of membrane and the pressure driving force.

Your R&D department has developed a novel membrane that has the potential to separate propylene and propane. These results have only been verified at the laboratory scale and the base-case results are contained in the table below.

Table 2 Membrane Data (Hayashi, 1996)

Temperature (^{o}C)	Selectivity (propylene/propane)	Propylene Permeance (g-mol•m^{-2}•s^{-1}•Pa^{-1})
100	33	2.9×10^{-9}
65	38	1.5×10^{-9}
35	46	7.9×10^{-10}

Using the data provided in the above table and information in the open literature, design a process to meet polymer-grade purity for the two sizing bases above (Table 1). This may incorporate a hybrid system using conventional distillation and membrane technology. Since Table 2 shows a relationship between operating temperature, selectivity, and permeance, determine the optimum operating conditions to maximize profit. Compare capital and energy costs of your design to conventional distillation. Some assumptions in the cost comparison are:

Steam costs $8/MMBTU
Electricity costs 6 ¢/kWhr
Cooling water costs 10 ¢/Mgal, and is available at 85ºF supply, not to exceed 105ºF return

Your management would like to know what membrane price to charge ($/ft^2) in order to make this an attractive investment for the end-user. You will also need to consider in your cash-flow analysis the maintenance and replacement costs for your membranes, expected to have a useful life of 2-5 years. Compare your price to commercially available membranes. Do a sensitivity analysis on membrane performance (flux rates and selectivities) as they would affect this market entry price, which will be used to develop targets for the commercial membrane product.

Finally, determine how your membranes might be used in an existing conventional distillation unit as a capacity debottleneck. For this economic evaluation, the steam-cracker clients value polymer-grade propylene at 1 ¢/lb above chemical grade propylene. Propane dehydrogenation clients value polymer-grade propylene at 15 ¢/lb above propane.

References

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Baker, R. W., *Ind. Eng. Chem. Res.*, **41 (**2002) 1393-1411.

Chilukuri, et al., *Ind. Eng. Chem. Res.*, **46 (**2007) 8701-8709.

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9. Model-Based Control with Stochastic Simulators: Building Process Design and Control Software for Advanced Materials Processing Technology (recommended by Talid R. Sinno, U. Penn)

Many materials processing technologies require careful control of features that are microscopic in nature and are not well described by continuum (i.e. field-based) models. An example is thin-film photovoltaic (PV) technology in which a thin layer of light-absorbing material is deposited onto a substrate. The advantages of thin-film PV over more traditional wafer-based silicon PV are now being realized as light-to-electricity conversion efficiencies become higher and processing technology improves, lowering cost. Examples of thin-film PV materials are Cadmium-Telluride (CdTe), Copper-Indium-Gallium-(di)Selenide (CIGS) [1], and silicon (Si) [2]. These materials are most often deposited onto glass or metal substrates, with typical film thicknesses being on the order of one to several microns. Controlled parameters of interest in such deposition processes are surface uniformity (i.e., roughness), porosity (void content), crystallinity (ordering extent), and chemical composition fluctuations (in multicomponent cases).

The goal of this design project is to utilize existing software for atomic simulation to develop a model for a deposition reactor that can be embedded into a model-based control (MPC) framework. The project will take advantage of the SPPARKS Monte-Carlo code (http://www.cs.sandia.gov/~sjplimp/spparks.html), which has been developed recently at the Sandia National Laboratory. This software allows the user to specify generic physical laws for describing the growth of a thin film onto an existing substrate. Shown in Fig. 1 is a schematic representation of some of the different atomic events that are carried out in a deposition simulation [3].

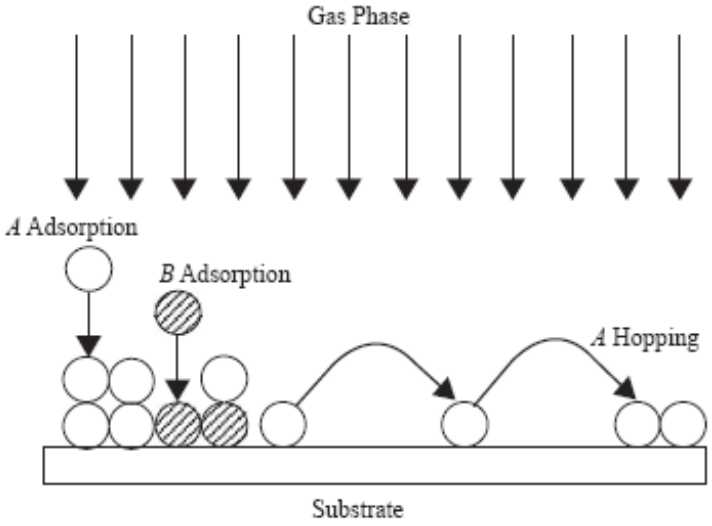
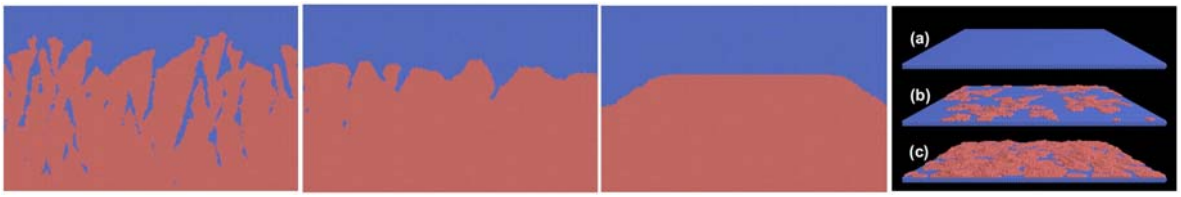


Figure 1: Schematic representation of atomic events that can occur during a simulation of a generic deposition process involving two different chemical components.

Specific Aims of the Design Project:

1. In the first part of the project, you will construct simulations of a generic deposition process in order to familiarize yourself with the SPPARKS code. The goal here will be to develop a quantitative understanding of how different process parameters such as temperature, deposition rate, and initial substrate texture affect the various deposited film properties, such as roughness, film porosity, and if possible, compositional distribution in a multicomponent system. Once these relationships are established you will use examples taken from the literature to build more realistic deposition models that correspond (approximately) to specific material systems; one example can be found in ref. [2], although others are readily available and can be considered instead. Example film configurations generated using the SPPARKS code for different deposition conditions are shown below for the specific case of crystalline nickel (taken from the SPPARKS website).



2. The second phase of the project will be to embed the SPPARKS code into a model-predictive control framework so that film parameters can be controlled dynamically during the growth of the film. The control algorithm will be implemented by writing a simple code (in a language such as C or Fortran, for example) that interfaces with the SPPARKS code via a script. The final product of the project will be an integrated piece of software, based on the SPPARKS engine, for modeling dynamically-controlled deposition processes.

3. Finally, using your software product, you will present a case study for an example deposition process in which the process parameters are optimized by balancing cost (generally specified by the throughput of your product) and film quality (which is dictated by the parameters specified above).

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10. Removing the Personal Medicine Bottleneck: $100 Genomes using Raindance Tech. (recommended by John C. Crocker, U. Penn)

The first human genome was published in 2003, and was the result of over $3 billion of public funding for the Human Genome Project (HGP). Around the same time, a privately funded company, Celera Genomics, using superior technology, published its own genome for just one-tenth the cost: $300 million. The content of a single human genome has immense utility as a research tool for understanding the molecular origin of disease. Currently, many researchers are focused on even a greater opportunity and technical challenge—personalized medicine. If the specific genome of an *individual* is known, then it can be used to predict their future predilection for different diseases, or to tailor more effective life-saving therapies for them, e.g., for cancer.

One impediment to personalized medicine is the current high cost of genotyping: you can have your complete genome sequenced today commercially [1], but it comes with a price-tag of $350,000. To stimulate further progress, in 2006 the X Prize Foundation announced the *Archon X Prize for Genomics* [2], which will award $10 million to the first team to sequence 100 different human genomes, for less than $10,000 apiece, in less than 10 days, with an error rate below ten per million bases. Several firms have started working toward the challenge, including *454* Life Sciences, Pacific Biosciences and Helicos Biosciences [3]. These companies make frequent reference to the '$1000 genome' and are expected to make the first X Prize claims any day now.

While these whole genome technologies are exciting, a larger impediment looms to threaten the idea of personalized medicine—*a complete lack of clinical data*. In total, only a few dozen genetic polymorphisms that interact with clinical treatments have been discovered to date, and sequencing just those polymorphisms costs a negligible amount. The most basic assumption of personal medicine is that if we had a large enough data set of whole patient genomes, we could discover millions of interactions between polymorphisms and clinical outcomes for different treatments via simple correlational data-mining. The central question is who will construct that dataset? The most plausible candidate is the large pharmaceutical companies themselves. Today, dosage decisions and safety contra-indications for pharmaceuticals are based on large data sets formed during clinical trials, at a cost of ~$10,000 per participant. If the cost of producing a whole genome was reduced to a few hundred dollars, then complete patient genotyping could become a standard practice during all clinical trials; essentially piggybacking the construction of a personal medicine database on the existing infrastructure.

This project is to design a '$100 genome' process within the context of a small startup company using the microfluidic emulsion microreactor technology commercialized by Raindance Technologies [4]. Raindance founder David Weitz has disclosed internal estimates that suggest per genome costs as low as $30, or *seven orders of magnitude cheaper* than the Celera technology of a decade ago. The team's business model will be a service company, receiving large numbers of patient samples (e.g., cheek swabs) from a pharma company client, and the electronic delivery of the corresponding whole genome data to the client within 30 days of sample receipt. Product sequences should have an error

rate of less than ten parts per million for non-repeating intronic sequences. The core (Raindance) technology consists of integrated fluidic systems that create, handle, combine and optically scan microscopic aqueous droplets flowing through oil-filled fluidic channels. Each droplet is in essence a tiny microreactor that can be used to perform the same biochemical assays conventionally performed at the lab bench with test tubes and pipettes, or on the well plate scale with automated fluid-handling robots. The tiny scale of the droplets dramatically decreases material costs, and allows higher throughput processing than possible for macroscopic robotics, single micro-devices can process 10^4 droplets per second.

The sequencing approach announced by Weitz's new startup GnuBio [5], and to be used as a baseline starting case by the team, is based upon the Watson-Crick base-pairing (hybridization) of a library of all 6 base oligonucleotides to roughly 1 kilobase (kb) fragments of patient DNA. By detecting which of the 4,096 oligos bind the patient fragment, it is possible to reliably reconstruct the fragment sequence using standard bioinformatic algorithms. To use this assay in a microfluidic platform, one will first have to create a library of droplets each containing just one of the 4,096 oligos along with a distinctive fluorescence 'barcode' identifier. Second, individual molecular fragments of patient DNA will be PCR amplified in large droplets (>1 nanoliter) that will then be broken down into thousands of smaller (~1 picoliter) droplets, each containing many copies of the original fragment. Third, these droplets will then be merged in a 1:1 fashion ('crossed') with the oligo library droplets. The merged droplets will be arrayed on a flat slide, and incubated to allow hybridization to occur in those droplets where the oligo finds a 6-base complementary section in the patient fragment. Hybridization will be detected by standard optical means such as Fluorescence Polarization (FP) or Fluorescent Resonant Energy Transfer (FRET). High throughput scanning of hybridization and droplet barcodes (to identify the oligo) will be required—Weitz estimates that existing CCD cameras and mechanical scanners should be able to effectively scan 10^6 droplets per second. Since the human genome contains roughly 3 billion bases, many millions of 1 kb patient fragments will need to be sequenced in this way, and then stitched together using other bioinformatic algorithms into a full sequence.

Like all whole genome sequence schemes, the Weitz/Raindance approach must minimize capital (for scanners), maximize throughput (minimize droplets scanned per sequenced base) and have an effective barcoding scheme (that simplifies scanning). In addition to analyzing the GnuBio strategy, the design team will also devise and investigate other sequencing/scanning approaches. For example, to minimize the number of droplets that must be formed and arrayed, one approach is to sequence entire fragments in each droplet via the optical readout of synchronous base additions, such as in the Helicos sequencing technology. In this approach [6], bases are added to a daughter strand one base at a time by a polymerase, with external synchronization of polymerases using an acid or UV cleavable modified nucleotide. This should allow many bases of sequence to be read out per droplet, as well as eliminate the need for any barcoding whatsoever, greatly simplifying and speeding scanning. To reduce capital costs associated with cameras and mechanical scanners (identified as challenges by earlier Penn design teams), one idea is to use a microfluidic substrate resembling a DVD that can be sealed after loading, rotated at high

speed and read out by a simple 'point scanning' optical head. While such a design process is potentially rather open-ended, it is expected that the team will quickly settle on a single most attractive sequencing approach. The team's approach and the Weitz/Raindance approach will then both be subjected to more intensive analysis and comparison of costs/throughput. An emphasis will be placed on process design to optimize sequence throughput as well as relevant biochemical reactions/kinetics, microfluidic fluid mechanics/network layout and fluorescence signal to noise, as all limit and determine ultimate throughput and cost. All sequencing approaches will need to be validated by bioinformatic reconstruction of mock data, most likely using the bioinformatics toolkit in MATLAB. Some of the raw data will contain errors due to finite signal to noise in fluorescence measurements, and the team will need to verify that these errors can be weeded out robustly to allow a final error rate of less than 10 parts per million in the final product sequence.

Since winning an X prize is not an acceptable business model, the team will evaluate the viability of a small venture capital funded biotech start-up, serving large pharma companies as their clients. The team will assume a Series A funded period in which the technology is demonstrated at a scale comparable to the X prize rate—10 genomes/day * 250 days/year = 2,500 genomes/yr. The team will determine their market price per genome based upon their own incremental and capital costs, as well as those estimated for their two closest competitors, but this is expected to be in the $100-300 range. After Series B funding, the assumed throughput with be quadrupled to 10,000 genomes per year. The financial analysis should seek a significant, positive NPV over a total four-year time horizon with an appropriate IRR for a biotech startup with VC funding. Acceleration of genotyping volume can be considered if market analysis suggests adequate demand. If the overall financial analysis looks favorable, the team should also estimate the capital requirements to expand their operational throughput to a plausible ultimate demand (after the widespread adoption of personalized medicine) of 10^6 genomes/year.

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11. Electrical Energy Storage Using Fuel-Cell Technology (recommended by Raymond J. Gorte, U. Penn)

Reversible fuel cells are potentially useful to store electrical energy due to good storage-scalability. There have been concerns over *round-trip* efficiency. This project will consider two types of fuel cells that utilize two different feeds. The two concepts will be compared for economic viability. Your team is to design the two systems and detail the pros and cons of each.

Electrical energy storage has a number of well-known applications for improving the ability of the electrical-grid to respond to demand fluctuations. The need for storage has become more acute as increasing amounts of intermittent renewable electrical sources become available. Examples are solar and wind turbines that produce electrical energy for only parts of the day – and not always during the same time periods. Consequently, it is difficult to match fluctuations in supply and demand. Ability to store electrical power becomes key to maintaining continuously-available energy as needed. The challenge is to store energy over extended periods and on a large scale. Consider that a utility company generates power from conventional and renewable sources. Also, let all of its power generated from green sources be utilized during the peak period from 7 AM through 7 PM. Green power generated during the other 12 hours can be stored for use during the peak period, with conventional (expensive) power reduced or shutdown during the peak period.

The first type of reversible fuel cell will have cells comprised of dense zirconium tubes or other configurations coated with doped $LaMnO_3$ for the air electrode (cathode) and using a porous Ni electrode (anode) on the fuel side. During electrolysis, a mixture of H_2O and CO_2 will be fed to the anode which carries out the half-cell reactions:

$$CO_2 + 2e\text{-} = CO + 2O^-$$
$$H_2O + 2e\text{-} = H_2 + 2O^-$$

Electrons will be supplied to the anode at a potential sufficient to drive the oxygen ions into the electrolyte. After the ions pass through the electrolyte, O_2 will be produced on the cathode via the other half-cell reaction:

$$2O^- = ½\ O_2 + 2e\text{-}$$

Note that during electrolysis, the overall heats of reaction are:

$$H_2O = H_2 + ½\ O_2 \qquad \Delta H(800ºC) = 248.3\ KJ/mole$$
$$CO_2 = CO + ½\ O_2 \qquad \Delta H(800ºC) = 282.4\ kJ/mole$$

However, the overall Gibbs energies of reaction, ΔG, which are equivalent to the standard potentials, are more relevant than ΔH. This process produces O_2, H_2, and CO, and requires electrical energy. The H_2 and CO and unreacted H_2O and CO_2 are stored to be available for the reverse reaction – when power is required during the peak period.

Either stored O_2, or alternatively air, can be used to produce electrical energy and convert the CO, and H_2 back to H_2O and CO_2. Your team is to decide whether to store O_2 or utilize air – at some loss in efficiency.

Consider a typical periodic source of 1 MW electrical energy availability (from 7 PM – 7 AM). Design a system to convert and store the energy.

The second type of reversible fuel cell is comprised of similar materials, but involves liquid Sb and Sb_2O_3, with outside storage likely required. It operates at ~700ºC – to be adjusted as a design variable.

The anode reactions are replaced by:

$$Sb_2O_3 + 6e- = Sb + 3O_2-$$

No electrode material is required, since Sb is conductive.

The Sb_2O_3 floats above Sb. The vessel containing the mixture holds the total system, possibly comprised of multiple vessels. For the reverse reaction and production of electricity, Sb_2O_3 passes through the zirconium system and converts Sb to give up electrons.

References

Fuel Cell Handbook, DOE/METC-94/ 1006

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12. Development of a High-Throughput System for Testing New Membrane Materials for Sterile Filtration
(recommended by Matthew J. Lazzara, U. Penn)

The sterile filtration of macromolecules and small molecules is critical to preparative processes in numerous biotechnology and pharmaceutical applications. Filtered molecules may include proteins with variable shape and charge properties, plasmids, and small-molecule drugs. In all cases, the Federal Drug Administration sets strict limits on the purity of the filtered product.

During the course of membrane operation, materials (including the desired product to be retained) can be deposited on membranes in a number of different ways (e.g., caking, pore clogging) which decrease the effectiveness and filtration capacity of the filter. In general, these membrane fouling processes and the performance of the filtration process are affected by a number of process parameters, including the composition of the mixture to be filtered, the material properties of the filter used, and the rate of filtration. Identifying the optimal operating conditions for a new filtration process can translate into significant cost and time savings in the downstream purification of therapeutic molecules.

Your task is to design a high-throughput system to test membrane filtration conditions in parallel in order to improve the ability to identify optimal operating parameters for the filtration of proteins, DNA, and small molecules. Your system should allow you to minimize the materials used to test individual conditions and maximize the number of conditions which can be tested in parallel. The process you develop should allow you to monitor the filtration of a relevant therapeutic molecule as a function of time, as well as all relevant process operation parameters.

In addition to developing the instrumentation for this process, you are tasked with developing analytical models for interpreting the filtration data to make accurate statements about the sieving coefficients characteristic of a particular combination of operation parameters. You will also develop the model necessary to translate your findings on the bench scale to predictions of membrane performance for industrial scale filtration devices.

In designing this high-throughput system, your design group will consider the possibility of creating a "small start-up" scale company/facility to optimize the performance of membranes for filtration of specific mixtures. Possibly your company will license the high-throughput screening product and/or create a facility in which it receives mixture samples from companies and carries out performance optimizations.

<u>References</u>

Microfiltration papers.

Specific references will be recommended in the near future.

13. Drinking Water Supply System using Concentrated Solar Power (CSP) with Stirling Heat Engine
(recommended by Adam A. Brostow, Air Products and Chemicals, Inc.)

When the Romans attacked the Greek port of Syracuse in 213 BC, Archimedes was said to have used mirrors to set the Roman ships on fire. In 1973, Greek engineer Ioannis Sakkas gathered 70 sailors at the port of Athens, each carrying a 1 × 1.5 m mirror. Collectively, they reflected the sun to one point on a mockup of a wooden Roman ship 50 m from the shore. The ship caught fire within three seconds. The combined effect of the 70 mirrors was equivalent to that of a single 100 m^2 parabolic mirror – providing concentrated solar power.

This design project involves two *Engineers Without Borders* (EWB) projects being carried out by its MAP (Philadelphia) Chapter. One is in Apatut, the Philippines, and the other is in Las Delicias, El Salvador. These are described next.

Apatut, the Philippines

This is a grass-roots project whose objective is to supply clean water to a village. Figure 1 shows a schematic of an elevation diagram in which a 20,000 gal tank sits 180 ft above Apatut. The elevation change from a pump at the bottom of a well to the top of the tank is ~350 ft (assumed to be 400 ft to overcome frictional losses). The water demand is 30 gpm (assuming 30 gal/person/day). The power from the grid is 220 V, 60 Hz, single-phase AC. The pump is likely to be submersible.

To supply water to Apatut, the design involves selecting the pump, calculating the power requirement, and selecting the energy source. If solar energy is the primary energy source, it will require energy storage. Alternatively, it may supplement energy from the grid to reduce the power cost to the village.

Las Delicias, El Salvador

This project involves improving an existing system. As shown in Figure 2, a submersible pump transfers water from the well to an intermediate tank. Then, a booster pump distributes water between two storage tanks at different elevations. Tank 1 holds 34,900 gal and tank 3 holds 25,350 gal. The distances, PVC tubing sizes, and the number of elbows are also shown. In addition, performance data are summarized in [1]. Some unknowns remain to be investigated.

The piping system will be modeled, possibly using ASPEN PLUS, and optimized assuming the use of a variable frequency drive (VFD). The usage of solar energy to drive the pump(s) or to supplement power from the grid will be considered. Note that power cost is a significant burden on the village of Las Delicias.

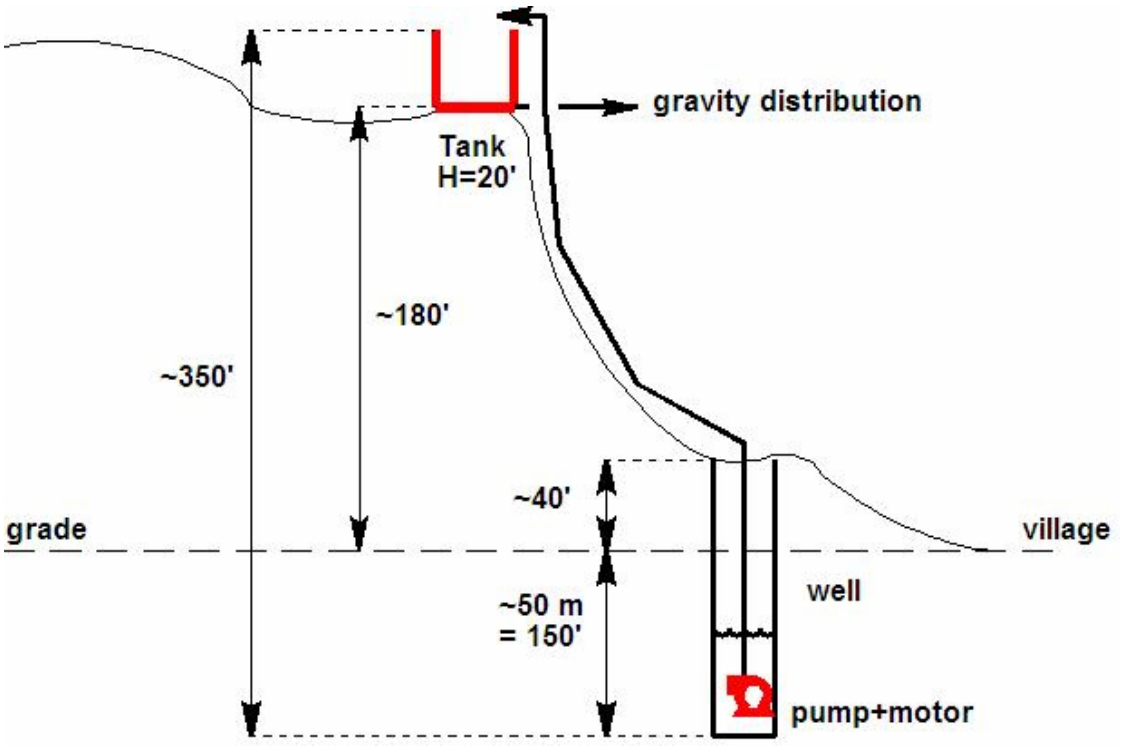

Figure 1. Apatut critical elevation diagram

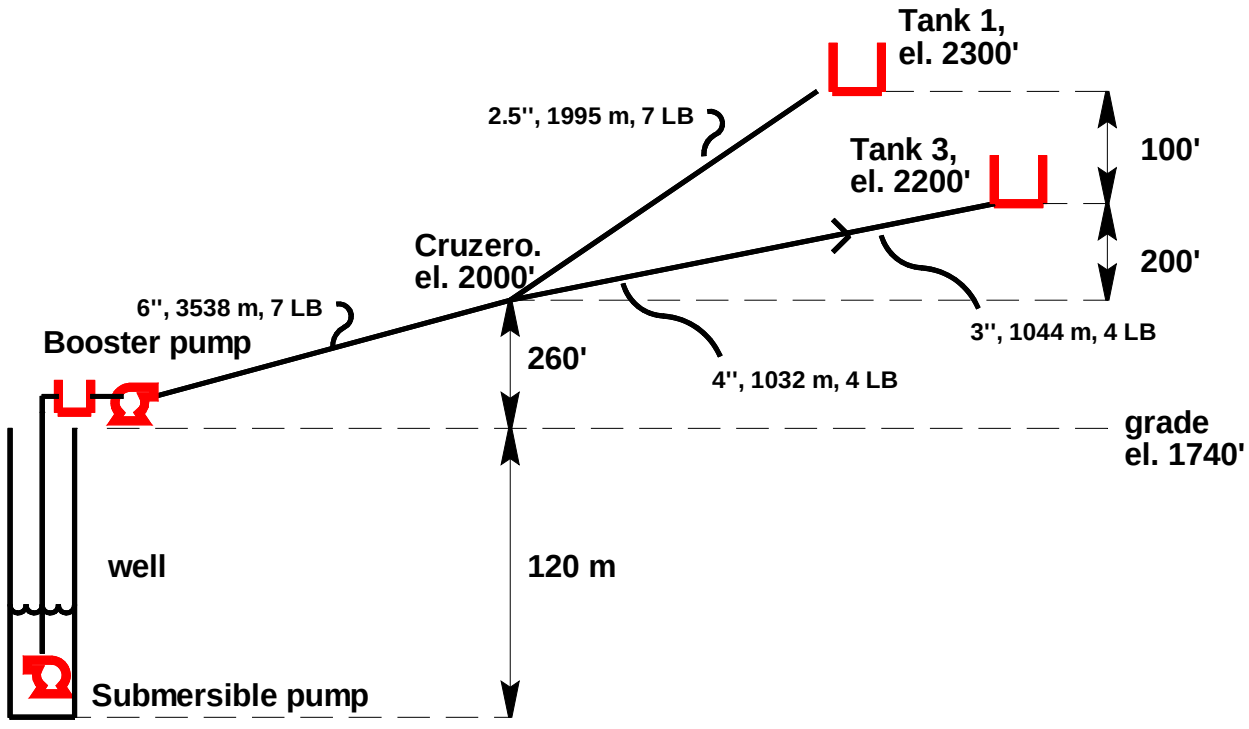

Figure 2. Las Delicias critical elevation diagram.

This design project will consider usage of the following solar energy sources:

- Conventional photovoltaic (PV) cells with optional energy storage
- Parabolic dish solar concentrator with Stirling engine and generator
- Multi-faceted parabolic solar concentrator with Stirling engine and generator
- Concentrated PVs using a parabolic dish, parabolic trough, multi-faceted parabolic solar concentrator, or High Gain Solar (possibly, to improve PVs in cloudy weather)
- Other promising sources

The design group will compare the economics, or at least the feasibility and practicability, of the different options and recommend the best solution. The possibility of constructing a working prototype should be considered. The Apatut and Las Delicias projects permit a comparison of designs to satisfy significantly different power requirements.

References

1. Analysis2.doc (describes the Las Delicias pumping system analysis)

2. MPSC.pdf (describing multi-faceted parabolic solar concentrator)

3. Solar Power: http://en.wikipedia.org/wiki/Solar_power

4. Solar thermal energy: http://en.wikipedia.org/wiki/Solar_thermal_energy

5. Concentrated solar power: http://en.wikipedia.org/wiki/Concentrated_solar_power

6. Stirling engine (including one directly driving a pump):
   http://en.wikipedia.org/wiki/Stirling_engine

7. High gain solar 100 (Concentrated PVs):
   http://www.technologyreview.com/energy/26003/
   http://www.skyline-solar.com/architecture.htm

8. 3M solar mirror films:
   http://buildaroo.com/news/article/3m-thin-mirror-films-for-solar-utility-applications/

9. Creative Science Center: http://www.creative-science.org.uk/parabola.html

10. El oro solar y otras fuentes de energía (La Ciencia Para Todos):
    http://www.amazon.com/solar-fuentes-energia-Ciencia-Spanish/dp/9681668928

14. Reclamation of Co-Solvents from Machined, Metal-Working, Cleansing Facilities (recommended by Leonard A. Fabiano, U. Penn)

Your company, Creative Tollers of America, has been asked to study and prepare proposals to recover co-solvents and reject the removed oil-water mixture from spent metal-working cleansing fluids. Also, the oil used in machining must impart its lubricating properties so that friction between the moving parts and the contact surface of any cutting tool is reduced (Forbes, 1943). From an OHSA perspective, a high percentage of water in the emulsion prevents the oil from misting into the atmosphere, exposing operators to potentially hazardous materials. As a result, the part being machined has a working surface that contains an inorganic contaminant, water, and an organic contaminant, oil. The overall cleansing strategy is to use an alcohol to remove the water and an organic solvent to remove the oil. Examples of the machined metal parts are those cut to a specific geometry – bearings, drawn tubes, or coils for heat-exchange equipment. The aircraft and rocket production industries also utilize large baths to clean oil and water from the parts' surfaces.

Mineral and vegetable oils are used in machining emulsions. The most commonly used mineral oils are refined paraffinic (C_nH_{n+2}) or naphthenic (C_nH_n) oils (Natchman and Kalpakjian, 1985), which are characterized by API gravity, viscosity, and flash point. Vegetable oils, on the other hand, consist of fatty acids and are used for their profound effect on the surface tension of water. Oleic acid or 9-octadecenoic acid ($C_{18}H_{34}O_2$) is a good example of a vegetable oil used in machining and will be used in this project.

In recent years, environmental concerns and laws have changed the choices of solvents. As a result, TCA and CFC-113 are now banned substances and have since been replaced by regulated solvents such as perchloroethylene (PCE), trichloroethylyene (TCE), HCFCs, and volatile methyl siloxanes and terpenes in aerosol form. However, with ever growing legislation, cleaning manufacturers and their customers often find managing regulated solvents like PCE and TCE a difficult task riddled with headaches. Thus, there has been recent interest in the use of non-regulated and/or more environmentally-friendly solvents like n-propyl bromide (NPB) and inseparable isomers of methoxy-nonafluoro-butane ($C_4F_9OCH_3$) or hydrofluoroethers (HFEs). NPB is a non-regulated solvent with cleaning capabilities similar to TCE and PCE. However, it is not clear how long NPB will remain a non-regulated substance. HFEs, on the other hand, are a class of compounds marketed by the 3M Company (1996 – reference not available) more as rinsing agents than as solvents since they are often mixed with trans-1,2-dichloroethylene and sold in a variety of non-azeotropic and azeotropic co-solvent cleaners. Isopropyl alcohol (IPA) has long been an accepted cleaning reagent in the medical industry and for water removal.

Nowadays the cleansing systems are vapor-phase degreasing processes. That is the contents of the degreasing equipment are maintained at typically 180ºF, depending on the co-solvent, in this project case. The degreasing equipment ranges from 4 to 80 feet long, with the smallest unit holding 100 gal of co-solvent and the largest unit containing four 4,600 gal truck loads. The vapor rises to envelop the metal parts and remove the oil from the metal surfaces. The effluent vapor rises to chillers for condensation, with the liquid recycled. The metal parts are cleansed while moving through the process at an elevated

temperature, emerging completely dry. The design and operation of the degreasing equipment to minimize or eliminate fugitive emissions is the responsibility of the cleaning system operations organization. Note: the reclamation company does not operate the onsite cleansing equipment. Their only goal is to clean up and resell the solvents.

The co-solvent mixture is initially at 56 mol% IPA and 44 mol% NPB, as this mixture has been determined to have superior characteristics/properties. During processing, after the co-solvent composition is reduced to 85 mol%, with 7.5 mole% oil and 7.5 mole% water, the resulting mixture is ready to be processed. Note that the initial clean co-solvent is always at a fixed purity. It is expected that the paraffinic oil, oleic acid, can be removed completely. Your company must decide the extent to which the water content can be lowered – to keep the equipment and operating costs reasonable. However, the water composition should not exceed 2.5 mol%.

Design a process to recover the co-solvent, NPB/IPA, from a degreasing system that requires one tank truck (4,600 gal) of fresh co-solvent. Typically a batch of co-solvent can be used for two weeks before the threshold of 15 mol% oil/water is reached. Note that the return mixture will contain 15 mole% oil/water. Your management requests that you consider a batch process, a continuous process, and a combination of the two. Determine the processing capacities at which the batch and continuous processes are economical. Does the combined process offer economic advantages? Is there a capacity below which only batch processing should be considered?

The Parts Cleaning Technology Company in Cinnaminson, NJ, should be of interest. Its facility provides fresh co-solvent to customers. It collects and sends the recycled mixture to its complex in Charlotte, NC, for recovery. It also has a facility in Bowling Green, KY, that manufactures cleaning equipment. Its website provides much general information: http://www.partscleaning.net/equipment.htm.

Given this collection point in Cinimminson, NJ, it seems clear that many local users need their co-solvent to be reclaimed. Suggest a good location for our proposed tolling operation. Steam, electricity, and cooling water utilities are needed. A location in the vicinity of a steam generation plant for the purchase of steam "over the fence" would be preferable to buying a steam-generation facility. It should be possible to make the other utilities available on site, along with process air and nitrogen (purchased).

Parts Cleaning Technologies sells NPB at $2.10/lb. IPA prices in bulk need to be found. At this point, we anticipated that the oil recovered will be incinerated. It likely contains some solid residues. You can assume fuel value for the oil.

This project offers the opportunity to learn more about batch distillation and where its use in commercial operations. Professor Fabiano will provide detail instructions on the application and use of Aspen Tech's batch distilation software.

References

Forbes W. G., *Lubricants and Cutting Oils for Machine Tools*, Wiley, 1943.
Natchman, E. S., and S. Kalpakjian, *Lubricants and Lubrication in Metalworking Operations*, Marcel Dekker, New York (1985)