University of Delaware CHEG 432 Main Design Project 2022

Methyl Acetate Manufacture

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Your company is a major manufacturer of acetic anhydride, an important industrial acetylation reagent and the largest commercially produced carboxylic acid anhydride. It wishes to expand its capacity by building a new 500 MMppy acetic anhydride ($(Ac)_2O$) plant. Your company employs carbonylation technology for which the raw materials are methyl acetate (MeOAc) and carbon monoxide. MeOAc is primarily an intermediate with few end use applications so it is not available in sufficient quantity for your needs on the merchant market. Therefore, part of the anhydride plant must be a 375 MMppy methyl acetate (MeOAc) plant.

Methyl acetate is conventionally made by esterification of acetic acid (HOAc) with methanol (MeOH) over an acid catalyst. But, there is an alternative route in which methanol is first dehydrated to dimethyl ether (DME) and then carbonylated directly to methyl acetate. Since you will already have carbon monoxide on site, this is a viable option for you. Furthermore, recent advances in carbonylation catalysis promise improved economics for this approach. You have been tasked with sorting out which route to pursue and with developing a design package for commercialization.

First, you must evaluate the competing routes (esterification vs. carbonylation) for methyl acetate synthesis and recommend the preferred route. You are to base this on a preliminary economic analysis that includes developing process schematics with major equipment identified for both processes, ***spreadsheet*** level material and energy balances, preliminary equipment sizing and preliminary profitability metrics.

MeOAc is generally synthesized for captive use, so there is no established selling price for it. In doing net present value analyses (NPV), you will look at the "net present cost" (NPC) for making the MeOAc by each approach and look for the approach that minimizes this cost. What this means is that you have no revenue stream, only costs associated with fixed and variable operating costs and the sunk investment of each route.

What your company will do in assigning profits to each operating unit is establish a "transfer price" for the MeOAc from the MeOAc plant to the $(Ac)_2O$ plant. This price will be such that the "internal rate of return" (IRR) will be 25%. Therefore, another approach to your economic analysis will be to compare transfer prices for each route calculated so that the IRR is 25%. The approach that minimizes NPC should also minimize the transfer price to the $(Ac)_2O$ plant ensuring that both the MeOAc facility and the $(Ac)_2O$ facility both have the best chance of earning an acceptable return.

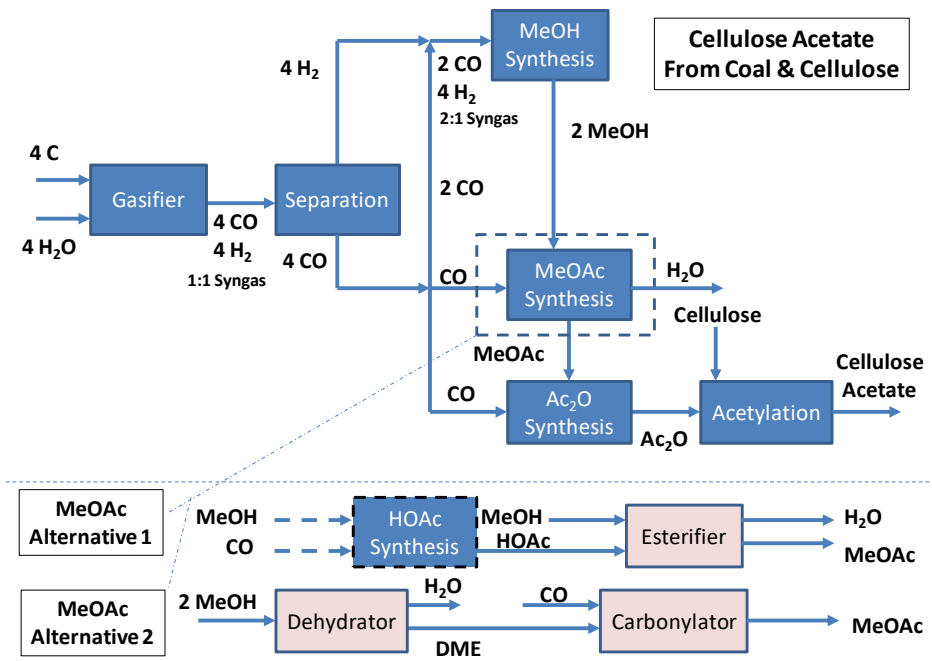
In a companion project, the recovery of DMAc from a waste stream, at least one of the alternatives under consideration will produce byproduct MeOAc. It is not clear that (a) this is the technology that will ultimately be adopted for that project, or (b) how much of your need could be supplied this way. But, those working on that project are valuing any MeOAc they produce at $1520/tonne. Based on your analysis, you should comment on whether or not you'd be interested in purchasing any byproduct from them at that price.

Having recommended a route, you will then proceed to the usual work of your process engineering group, namely, the development of a fully converged and profitability-optimized flowsheet using the Aspen process simulator, with equipment sizing sufficient to allow the plant to be built and venture guidance level profitability analysis (NPC and transfer price at 25% IRR).

CONTEXT

The major market for your acetic anhydride is the manufacture of cellulose acetate by acetylation of cellulose with acetic anhydride. The following figure shows a possible supply chain to cellulose acetate from coal and cellulose in which the coal is gasified with steam to make a 1:1 H_2:CO syngas which is separated into its components and then recombined as needed to enable synthesis of MeOH, MeOAc and Ac_2O. Your firm will own the MeOAc and Ac_2O portions of this supply chain. Someone else owns the

infrastructure producing CO, MeOH and HOAc. The MeOAc portion is shown as a block into which the two alternatives above can be dropped. Both alternatives are shown in the figure. The synthesis of HOAc is shown as part of the esterification alternative although in your conventional route plants, this is owned by others from whom you buy HOAc. It is shown to emphasize that the manufacture of MeOAc requires the same quantities of MeOH and CO, regardless of route, since HOAc is produced by carbonylation of MeOH. The choice of coal for illustration is based on having the right C/H/O stoichiometry when gasified with steam. In actual fact, the carbon may come from natural gas. This produces more H_2 than is needed for Ac_2O, but the excess could be used in other processes, for example ammonia manufacture.



BASIC DATA

Acetic Acid Esterification

The esterification of acetic acid (HOAc) with methanol (MeOH) to form methyl acetate is acid catalyzed, and your R&D chemists have identified a gel-form ion-exchange resin which acts as a solid strong acid catalyst for this reaction:

$$\text{MeOH(l)} + \text{HOAc(l)} = \text{MeOAc(l)} + \text{H}_2\text{O(l)}$$

Esterifications are well known to be reversible, so the reaction equilibrium must be included in the reaction rate expression. The reaction rate data is consistent with the following:

$$r_{ester} = k_{ester}\left([\text{HOAc}][\text{MeOH}] - \frac{[\text{MeOAc}][\text{H}_2\text{O}]}{K_{ester}}\right)$$

$$r_{ester} = \text{esterification rate, gmol/g}_{\text{catalyst}}\text{/min}$$

$$k_{ester} = \text{esterification rate constant, L}^2\text{ / gmol/g}_{\text{catalyst}}\text{/min}$$

$$K_{ester} = \text{esterification equilibrium constant}$$

$$[\text{X}] = \text{concentration of species X, gmol/L}$$

Development studies by your R&D department have shown that the forward rate constant for esterification is:

$$\ln k_{ester}\,(\mathrm{L}^2/\mathrm{gmol}/\mathrm{g}_{\mathrm{catalyst}}/\mathrm{min}) = 4.08 - 5400/T(\mathrm{K})$$

where T is the absolute temperature. Your company has used this catalyst in other esterifications so you know that it has a service life of 2 years as long as the reactor is operated at less than 100 C.

Methanol Dehydration

Ion-Exchange Resin Catalyst

Methanol dehydration to form dimethyl ether (DME) is the first step in the carbonylation route, but it is also a known side reaction of the esterification, so it must be considered there as well. This reaction is also reversible, although the equilibrium favors products more strongly than in the esterification reaction. High conversions are desirable for carbonylation, but in esterification, it is a yield loss and furthermore, produces water that will suppress the esterification equilibrium:

$$2\ \mathrm{MeOH}\ (\mathrm{l}) \rightarrow \mathrm{DME}(\mathrm{l/g}) + \mathrm{H_2O}(\mathrm{l})$$

DME is a low boiler and in the esterification route, significant generation will cause vapors to form that may interfere with efficient condenser operation in the downstream distillations. The kinetics of the dehydration over the ion-exchange catalyst are second-order and follow a Langmuir-Hinshelwood form with a rate-limiting step involving two active sites on the catalyst, where all the sites hold either adsorbed water or adsorbed methanol:

$$r_{dehy} = \frac{k_{dehy}\left(1 - \dfrac{[\mathrm{DME}][\mathrm{H_2O}]}{K_{dehy,l}\,[\mathrm{MeOH}]^2}\right)}{\left(1 + \dfrac{K_W}{K_A}\dfrac{[\mathrm{H_2O}]}{[\mathrm{MeOH}]}\right)^2}$$

r_{dehy} = MeOH dehydration rate, gmol/$g_{catalyst}$/min

k_{dehy} = dehydration rate constant, gmol/$g_{catalyst}$/min

$K_{dehy,l}$ = dehydration equilibrium constant in liquid

K_W = adsorption equilibrium constant for H_2O on catalyst

K_A = adsorption equilibrium constant for MeOH on catalyst

The literature (Gates, B. C., and Johanson, L. N., *AIChEJ*, **17**, 981 (1971).) gives the forward rate constant as:

$$\ln k_{dehy}\,(\mathrm{gmol}/\mathrm{g}_{\mathrm{catalyst}}/\mathrm{min}) = 24.3 - 12300/T(\mathrm{K})$$

and your R&D department has estimated the adsorption equilibria to be given by:

$$\ln \frac{K_W}{K_A} = 11.1 - 3300/T(\mathrm{K})$$

which is consistent with the values reported by Gates and Johanson at 106 C.

H-Mordenite Catalyst

Bondiera and Naccache (*Applied Catalysis*, **69**, 139-148 (1991)) report that the H-mordenite form of zeolite to be used in the carbonylation step also can catalyze MeOH dehydration to DME in the vapor phase above 250 C.

$$2\ \text{MeOH (g)} \rightarrow \text{DME(g)} + \text{H}_2\text{O(g)}$$

They report a 1st-order rate law in MeOH partial pressure, but ignore potential reversibility and also inhibition by both MeOH and water adsorption. It is likely that they made observations at low conversion and missed all of these effects as a result.

Your R&D department has made some additional measurements and suggest a modification of their rate expression as follows:

$$-r_{MeOH} = \frac{r_{DME}}{2} = \frac{r_{H_2O}}{2} = \frac{kK_{MeOH}}{1 + K_{MeOH}\,p_{MeOH} + K_{H_2O}\,p_{H_2O}}\left(p_{MeOH} - \frac{p_{DME}\,p_{H_2O}}{p_{MeOH}\,K_{dehy,g}}\right)$$

$$k = \text{forward rate constant}$$

$$K_{dehy,g} = \text{dehydration equilibrium constant in gas}$$

$$K_{MeOH} = \text{adsorption equilibrium constant for MeOH}$$

$$K_{H_2O} = \text{adsorption equilibrium constant for } \text{H}_2\text{O}$$

$$p_X = \text{partial pressure of species X, Pa}$$

The values of their rate parameters are:

$$\ln k\left(\text{kmol/kgcat/s}\right) = 28.809 - \frac{19743}{T(\text{K})}$$

$$\ln K_{MeOH}\left(\text{Pa}^{-1}\right) = -36.312 + \frac{10063}{T(\text{K})}$$

$$\ln K_{H_2O}\left(\text{Pa}^{-1}\right) = -25.212 + \frac{6763}{T(\text{K})}$$

In addition, they find that the catalyst temperature must be kept below 400 C to avoid excessive deactivation. So long as this requirement is met, you may assume a 2-year catalyst lifetime.
You are free to consider either of these catalysts for the dehydration step in the carbonylation route.

Dimethyl Ether Carbonylation

According to recent research (Cheung, et al., "Site requirements and elementary steps in dimethyl ether carbonylation catalyzed by acidic zeolites, *J. Catalysis*, 245 (2007) 110-123.), DME is carbonylated with high selectivity to form MeOAc over H-mordenite:

$$\text{DME} + \text{CO} \rightarrow \text{MeOAc}$$

After an induction period during which the zeolitic protons are displaced by methyl and acetyl species, this reaction appears to occur by the following mechanism:

CO + ^ = CO^

CO^ + CH_3* = CH_3CO* + ^

CH_3CO* + DME → CH_3* + MeOAc

The species CO^, CH_3* and CH_3CO* are surface intermediates and the symbols ^ and * represent two types of catalytic sites, one holding adsorbed CO molecules and the other holding the methyl- and acetyl-intermediates. The middle reaction is apparently rate controlling so that the adsorption of CO is at equilibrium and the overall rate only depends on the CO partial pressure. Overall, the reaction is irreversible. If any water is present, it competes with CO for adsorption on ^ sites and inhibits the reaction.

Under steady state conditions following proton displacement from the original acidic catalyst, the overall reaction rate is given by:

$$r_{carbonyl} = k_{carbonyl}\left(\frac{K_{CO}\,p_{CO}}{1+K_{CO}\,p_{CO}+K_{H_2O}\,p_{H_2O}}\right)$$

$$r_{carbonyl} = \text{carbonylation, gmol/g}_{\text{catalyst}}\text{/hr}$$

$$k_{carbonyl} = \text{carbonylation rate constant, gmol/g}_{\text{catalyst}}\text{/hr}$$

$$K_{CO} = \text{CO adsorption equilibrium constant, atm}^{-1}$$

$$K_{H_2O} = \text{H}_2\text{O adsorption equilibrium constant, atm}^{-1}$$

$$p_X = \text{partial pressure of species X, atm}$$

Apparently, the fractional coverage of CO on the ^ sites is low, so that this may be approximated as:

$$r_{carbonyl} = \frac{k_{carbonyl}K_{CO}\,p_{CO}}{1+K_{H_2O}\,p_{H_2O}}$$

Data in Cheung, et al. suggest that for DME-pretreated H-mordenite catalysts:

$$k_{carbonyl}K_{CO} = 3\times10^4\exp\left(-\frac{8370}{T(\text{K})}\right)\ \text{gmol/g}_{\text{catalyst}}\text{/hr/atm}$$

The denominator in the reaction rate expression is related to the fractional coverage of the CO-holding sites with water (θ_{H2O}) which effectively deactivates the catalyst. Zhu, et al. (*J. Membrane Sci*., **253**, (2005) 57-66.) show that this can be described by the Unilan isotherm which results in:

$$\frac{1}{1+K_{H_2O}\,p_{H_2O}} = 1-\theta_{H_2O} \quad\Rightarrow\quad r_{carbonyl} = \left(k_{carbonyl}K_{CO}\right)\left(1-\theta_{H_2O}\right)p_{CO}$$

where:

$$\theta_{H_2O} = \frac{1}{2s_{H_2O}}\ln\left(\frac{1+e^{s_{H_2O}}K^U_{H_2O}\,p_{H_2O}}{1+e^{-s_{H_2O}}K^U_{H_2O}\,p_{H_2O}}\right) \quad ; \quad K^U_{H_2O} = \text{Value of } K \text{ for water in Unilan equation}$$

with:

$$s_{H_2O} = \frac{1591}{T(K)} \quad ; \quad K^U_{H_2O}(\text{atm}^{-1}) = 478.3 \exp\left[19.856\left(\frac{340.6}{T(K)} - 1\right)\right]$$

Some calculations with these expressions will show how water-free the carbonylation reactor feed must be in order to avoid significant catalyst deactivation.

Feed Purity

You may assume that the MeOH feed is at least 99.9 wt% pure with the principle impurity being water at no more than 0.1 wt%. Since HOAc is made by carbonylation of MeOH, you may assume that your HOAc feed for the esterification route is 99.9 wt% HOAc with no more than 0.1 wt% MeOH. The behavior of these impurities is completely described by the chemistry already discussed in the foregoing sections.

For the carbonylation route, the CO feed arrives by pipeline with 0.5 vol% H_2 impurity at a pressure of 175 psig. Your R&D chemists have shown that the chemistry follows an Ely-Rideal mechanism in which H_2 interacts with species on the *-type catalyst sites as follows:

$H_2 + CH_3^* \rightarrow H^* + CH_4$

DME + H* → CH3* + MeOH

You will therefore need to address the potential for unreacted H_2 and byproduct CH_4 to buildup in gas recycles around the reactor and will need to clean up the product methyl acetate to meet the MeOH specification.

Your R&D department has measured the rate of this hydrogenation reaction and finds that it is described by:

$$r_{hydrogenation} = k_{hydrog}\, p_{H_2}$$

The rate constants can be expressed as a simple ratio to the carbonylation rate parameters:

$$\frac{k_{hydrog}}{k_{carbonyl} K_{CO}} = 1.7$$

Separations

It is expected that all separations can be done by distillation, but there are at least two azeotropes which must be considered: MeOAc/MeOH, and MeOAc/H_2O (both low boiling). MeOAc/H_2O and DME/H_2O also exhibit liquid immiscibility (the latter probably at elevated pressure). So… care must be taken in using the VLE data and models in standard process simulation packages. Some review and critique is in order. Some data on the above azeotropic compostions and miscibility gaps are given below and may be useful for thermodynamic parameter estimation:

MeOAc-MeOH Azeotrope

Tu, C.-H., Wu, Y.-S., and Liu T.-L., *Fluid Phase Equilib.* **135**, 97 (1997.)

P(mm Hg)	T(C)	wt% MeOAc
760.00	54.3	83.1

MeOAc-H_2O Azeotrope

Marshall, A., *J. Chem. Soc.*, **89**, 1350 (1906).

P(mm Hg)	T(C)	wt% MeOAc
777.21	56.9	97.2

Miscibility Gaps

T(C)	wt% MeOAc in MeOAc	wt% MeOAc in H_2O
20	92	23
40	90	23
60	86	23
80	82	28

T(C)	wt% DME in DME	wt% DME in H_2O
0	94	39
40	92	29

Product Specifications

If MeOAc is made by esterification of HOAc with MeOH, the specification is:

HOAc < 0.1 wt%	(can be separated and recycled to MeOAc synthesis)
MeOH < 0.8 wt%	(carbonylates to HOAc in $(Ac)_2O$ manufacture, see HOAc spec)
H_2O < 0.8 wt%	(hydrates $(Ac)_2O$ to 2 HOAc, see HOAc spec)
DME < 100 wt ppm	(doesn't carbonylate (different catalyst system for $(Ac)_2O$ synthesis) and requires vapor vents from condensers)

This specification results in once-through product that is approximately 95 wt% $(Ac)_2O$ and 5 wt% HOAc.

If MeOAc is made by carbonylation of DME, the specification is:

HOAc < 100 wt ppm	(HOAc unwanted – no value in MeOAc synthesis)
MeOH < 100 wt ppm	(carbonylates to HOAc in $(Ac)_2O$ manufacture, see HOAc spec)
H_2O < 100 wt ppm	(hydrates $(Ac)_2O$ to 2 HOAc, see HOAc spec)
DME < 100 wt ppm	(doesn't carbonylate (different catalyst system for $(Ac)_2O$ synthesis) and requires vapor vents from condensers)

This product should be more valuable because it doesn't add HOAc separations investment to the anhydride plant. You may want to consider the economic value of the avoided investment somehow in your economic analysis.

ECONOMIC DATA

For utilities, waste treatment, labor, maintenance and all other costs exclusive of raw materials, please refer to guidelines supplied by your professors. You may assume the following prices for your raw materials:

HOAc - $1720/tonne (1 tonne = 1 metric ton = 1000 kg)
MeOH - $620/tonne
CO - $205/tonne

You may assume that the ion exchange catalyst for esterification has a bulk density of 800 kg/m3 and sells for $4.90/kg. The H-mordenite zeolite catalyst has a bulk density of 610 kg/m3 and sells for $70/kg.

PRELIMINARY ECONOMIC SCREENING WITHOUT A SALES PRICE

Using the net return on investment metric (NROI), you can do some preliminary economic screening just based on these ingredients costs, with no knowledge of the required investment for either route, except perhaps a block flow diagram indicating how many reactors and columns you think are needed for each process and a consideration of the materials of construction for the two routes. The following equation is a starting point:

$$NROI = \frac{(1-t)(R - AC - VC - FC)}{FI + WC}$$

$$\begin{aligned} NROI &= \text{net return on investment, fraction} \\ t &= \text{tax rate, fraction} \\ FI &= \text{fixed investment, \$MM} \\ WC &= \text{working capital (inventories), \$MM} \\ R &= \text{revenue, \$MM/yr} \\ AC &= \text{administrative costs, \$MM/yr} \\ VC &= \text{variable costs, \$MM/yr} \\ FC &= \text{fixed costs, \$MM/yr} \end{aligned}$$

You may assume a typical tax rate is 0.25 (25%) and since your target IRR is 25%, you should assume that the target NROI is 0.25. Furthermore, you can make some assumptions that allow you to estimate many of the rest of these quantities. Note that these are preliminary estimates only and not suitable for final project economics. Nevertheless, this type of preliminary screening analysis shows you what the economic landscape looks like.

Since raw materials costs usually dominate variable costs, ignore energy costs for now. Even if you get substantially less than 100% per pass through the reactor, you will generally engineer the process to recover and recycle as much unconverted raw material as possible. Unless you know that side reactions are a major loss pathway, it is reasonable to assume 100% yield at this point. This means that you can make a preliminary estimate of variable costs from raw materials prices:

$$VC = \underset{\text{ingredients cost at 100\% yield}}{IC_{100}}$$

Fixed costs can be approximated as 14% of the fixed investment plus labor costs. Labor costs, including supervision and overheads are approximately equal to \$0.8MM/yr/operator/shift. The number of operators you need per shift is 1 to man the control board and 1 field operator for each process area. A rule of thumb might be that a process area is 2 major pieces of equipment, e.g., a reactor and a column or 2 columns. Then:

$$FC = .14FI + \$0.8\text{MM/yr} \times \underset{\text{operators/shift}}{n}$$

You can estimate administrative costs as 6% of the mill cost which is equal to variable plus fixed cost:

$$AC = .06(VC + FC) = .06\left(IC_{100} + .14FI + \$0.8\text{MM/yr} \times n\right)$$

To calculate working capital, inventories of raw materials are valued at purchase cost and product is valued at mill cost (*VC*+*FC*). A typical assumed inventory is 1 month of each raw material and product, so:

$$WC = \frac{VC}{12} + \frac{VC + FC}{12} = \frac{VC}{6} + \frac{FC}{12} = \frac{IC_{100}}{6} + \frac{.14}{12}FI + 0.067\$\text{MM} \times n$$

This means that everything on the RHS of the NROI equation has been estimated in terms of IC_{100}, *FI* and *n* except for revenue (*R*). Since there is no selling price for MeOAc, this becomes a variable in the screening analysis. The prices allow you to calculate IC_{100}, and block flow diagrams allow you to estimate *n*. Therefore, the NROI equation gives you a relationship between *R* and *FI*.

You also don't know how the investments for the alternate routes compare. This gives you a parameter you can vary to develop a family of curves. For example, you can define this parameter as the carbonylation-to-esterification fixed investment ratio. Then you can vary fixed investment for the route with the cheapest ingredients while maintaining this investment ratio (i.e., the other processes investment varies also according to this ratio) and calculate the required revenue to earn 25% return for both processes. Dividing by the production rate gives a value of the transfer price for each route to earn 25% return. Taking the difference in transfer prices and plotting versus the investment you used as the independent variable should give you a curve that crosses the x-axis at some investment value. This defines a critical investment value below which one process is preferred and above which the other one is.

Doing this for multiple values of the investment ratio generates a family of curves and a locus of these critical investment values. You will find that this locus is a hyperbola with the vertical asymptote occurring at an investment ratio of 1 (both processes have the same investment). You can find the horizontal asymptote by setting the investment in the process with the more expensive ingredients to zero and finding the revenue at 25% NROI. Then find the investment in the process with the cheaper ingredients that generates this same revenue at 25% NROI.

This pair of graphs will give you a nice map of the economic space. You can then look at your block flow diagrams and expected materials of construction and make some guesses about the likely value of the investment ratio and see where it locates you on these graphs. As you develop insight into what the likely investment will be in either route, you will be able to make an early determination of which one is preferred. The sooner you reach this point, the more you can concentrate on fully developing the preferred route.

PROJECT SCHEDULE & DELIVERABLES

Thursday, 3/17 - 1ST PROGRESS REPORT

Deliverables:

1. Preliminary screening analysis based on ingredients cost and the analysis approach described in the writeup
2. Process block diagrams for all routes that pass the preliminary screen
3. Spreadsheet level material and energy balances for these routes

Comments:

Material and energy balances are to be crude at this point. You should have completed Douglas steps 1 and 2 (batch vs. continuous assessment and input-output structure identification) and be starting on Douglas steps 3 and 4 (recycle structure and separation systems structure). You should apply the Level 0 technique (as modified in the writeup when no selling price is known) in which you develop maps of the economic space. You should consider identifying how many reactors and columns each approach will take and their likely materials of construction so that you can get an early gauge of what the likely ratio of investment will be between the two routes. Assume conversions and reflux ratios, only look at major energy consumers, don't worry about converging minor components. You should be able to do all of this without using Aspen. Are you able to decide on a route? If not, which way are you leaning?

Thursday, 4/7 - 2nd PROGRESS REPORT

Deliverables:

1. Recycle & Separations Structure
2. Back–of–envelope economic analysis for all routes still under consideration based on:
   - Preliminary equipment sizing and investment estimate (VGA)
   - Preliminary COM (cost of manufacture)
   - Preliminary Transfer Price and NPC (4/10 edit, can't hold students to it, did say NPV in original write up – There are several bases for establishing Transfer Price – either use Cost Sheet to find price at 25% NROI and then calculate NPV and IRR – or use NPV calculator to get Transfer Price (IRR will be 25%) and then calculate NROI)
3. If possible, finalize route selection

Comments:
You should have made at least one pass through Douglas steps 1-4 now for each route. Equipment sizing should be crude at this point using the short-cut methods you've learned. You are aiming to approximate the investment well enough to make decisions among alternatives, not well enough to justify authorization of the project. You want to narrow the choices before you invest a lot of hard work on really developing the flowsheet and doing a thorough job of equipment sizing. You only want to expend that level of effort on a few options. If you are continuing to work on more than one route beyond this point, you should be able to indicate how you hope to improve the less attractive routes so that they compete with the best one. Although Aspen simulation is not one of the deliverables for this Progress Report, you should have already begun working in Aspen with those routes you intend to carry forward.

Thursday, 4/21 - 3rd PROGRESS REPORT
Deliverables:
1. Complete Aspen flowsheets for at most two routes
2. Refined reactor designs
3. Refined economics (VGA, COM, NPC, Transfer Price, NPV, IRR)
4. Final recommendation on route.

Comments:
This is now the time to roll up the sleeves and really get into the details. You should be finalizing the recycle structure and separations systems structure. Your reactor designs should now reflect the reaction kinetics so that the Aspen flowsheet and the equipment sizing are internally consistent. In addition to a converged flowsheet, you must also indicate the disposition for every stream exiting the facility and ***qualitatively*** why that was selected. If you are recycling, demonstrate feasibility of recycle loops. No loose ends.

Thursday 5/5 - 4th PROGRESS REPORT
Deliverables:
1. Heat Integration
2. Final equipment sizing for chosen route
3. Final profitability analysis for chosen route (VGA, Cost Sheet, NPC, Transfer Price, NPV, IRR)
4. Sensitivity analysis indicating which variables have the biggest impact on profitability
5. Assessment of risk level in implementing chosen route and any strategies for mitigation

Comments:
You should continue to complete your design package at a more detailed level of equipment design. Now is the time to really figure out what reflux ratios should be and the tray number or packing height requirements for the columns. Now is the time to complete Douglas step 5 (heat & energy integration). Be sure to present economic results in standard formats for such things as investment estimates, cost sheets, discounted cash flow calculations.

Thursday, 5/12 - FINAL WRITTEN PROJECT REPORT
Clean up any loose ends from your previous work and apply the polish to prepare a formal report. The main points of your report are to:
(a) make your route recommendation for MeOAc sourcing,
(b) present the expected economics to the business and
(c) communicate a design package so that the business can authorize a capital project should this prove attractive.

In addition to covering the main points of all the evaluation, design and economics you've done, you should now include sections in your report addressing such things as environmental footprint, process safety and reliability and other social concerns of 2021.

Friday/Monday/Tuesday 5/13, 5/16, 5/17 - ORAL PRESENTATION
For your presentation, you will not be able to cover every aspect of your formal written report in detail. You should orient this presentation to convincing your audience of:
(a) your MeOAc route recommendation
(b) the quality of your design
(c) the believability of your economics