**Who/What/Where/When/Why/How**

The final project will be "delivered" as a code/report (insert results into template) and communicated to the entire class (including instructor, TA, and peers) during the scheduled final exam time slot.

The presentation will be aimed to be 5 minutes (results only) with 3-5 minutes of live/interactive Q&A.

The project itself will involve generating a cumulative Matlab code that does the following:

* creates a model (or various models) of a small mini chemical plant
* the plant will aim to produce highly purified acetic acid
* the plant will contain several types of reactors and purifiers (distillation, LLE, etc)
* the plant will have option to use various feed options, recycles, and more
* the plant will have to generate certain outputs and meet certain constraints

You will have your code solve for the optimal design and operating conditions for the plant based on the specifics to be provided for the above. At the end of the day you will be the CEO of the plant, and beholden to the shareholders, government regulators, and societal/public need. As with many engineering design problems, there is not necessarily always one single and correct universal answer to the problem. Your presentation will argue why your code/model is appropriate for your economic and moral needs and values, and demonstrate how outputs and profits change if your needs or values change.

# Template File for Final Project Presentation

Attached here. You are REQUIRED to use this.

Yes, it is plain and boring. I know that. It makes it easy to see exactly what I'm looking at/for consistently, which is key in the

short, rapid-fire session we will hold

# Recommended Workflow/Process of Attack

1) Read entirely of project background, plant specs, equipments, costs, etc .

2) Do some literature / reading on what are good catalysts for the reaction, good solvent(s) for the LLE, etc.

choose materials that meet YOUR social/ethical/safety/environmental concerns

3) Once chemicals/materials chosen, create modular UDF (User Defined Function) that characterize each piece of equipment.

Have them take inputs of structure variables (var.field1 etc) and output structure(s) or single variables as needed.

Example, batch reactor inputs could include operating temperature, amount of catalyst, concentration of feedstock, etc. Outputs would include time operated in batch, exit concentration, etc.

4) Link your pieces of equipment into an overall train and model the entire process given inputs (relevant) and output things like the overall exit concentration, purity, temperature, etc.

5) Create an optimization model that maximizes or minimizes #4 to basically do things such as use as little energy , or achieve highest purity, etc of interest to you.

6) Create an economic model that describes the operation of the plant, including some random generation for things like equipment failures or safety incidents per the terms of the problem statement(s). Add any other relevant constraints given or that you want to apply.

7) Solve the economic model in #6 to maximize your profits (even if you just want to give them to charity), subject to meeting the minimum required outputs.

8) Put your results into the (soon to be) provided template slides.

Be ready to explain your results, how your code works, and have it adaptable enough to be re-run on the spot if questioned about it.

# Plant Specs

Plant needs to, at a minimum\*

**produce the following**

10 tons of acetic acid per week, with 98.5% purity

**pay workers a competitive market salary**

**be as profitable as possible subject to moral/social constraints**

worker pay/quality of life

CO2 emissions

waste generation

overall sustainability

etc...

# Available Equipment

**Reactors:**

5x 100L batch reactors, which can make acetic acid via fermentation by bacteria or yeasts. These reactors are unjacketed (no temperature control). Any feeds or products entering/leaving must be preheated/cooled.

5x PBR or PFR reactors which can make acetic acid via carbonylation of methanol. 2 of the reactors are 10L capacity, 3 of them are 20L capacity. Each is jacketed. They all have the same Length: 2meters

**Separators:**

3x Continous Distillation Columns with Reflux capacity , variable feed trays, variable tray geometry, and jacketed temperature controls. Each column has a total volume of 10 cubic meters.

5x Liquid Liquid Extraction Columns, each with 50L capacity, variable tray/packing geometry, jacketed controls for temperature and vapor relief. Each column operates in the ternary acetic acid/water/????? system.

??? denotes theoretical LLE column/still integrated system that can handle any relevant ternary agent

<https://pubs.acs.org/doi/full/10.1021/acs.jced.1c00474>

[Links to an external site.](https://pubs.acs.org/doi/full/10.1021/acs.jced.1c00474)

https://en.wikipedia.org/wiki/Ternary\_plot

**PreHeaters/Coolers/Boilers**

You have as many of these as you need. They can operate with the costs , energy inputs, and CO2 outputs as specified in the "COSTS" page

Notes:

You can assume none of the LLE is kinetically limited. In other words, they operate at their Equilibrium Limits

You can assume ideal mixing of species where relevant

You can assume that Reactors can withstand any temperatures up to 500K, and pressures up to 10 atm. Anything beyond that will generate a meltdown or explosion safety event.

You can assume that there exist PID control systems to implement whatever operating conditions you have decided to run.

You can assume that the plant operates 24/7 (unless incident) , employees are on 8 hour shifts, and you need 1 employee per major piece of equipment in operation , 1 safety engineer per shift, and 1 overall plant supervisor per shift.

# Costs

Your feed stocks have the following costs:

Bacteria/Yeast/Fermenting Agent (AAB : Acetic Acid Bacteria, for example): $25/pound

aqeuous Ethanol: $10/gallon, 80 proof; $20/gallon, 100 proof; $30/gallon, 120 proof; $50/gallon, 150 proof

Water: $500 per 1000 gallons

Methanol: $3/gallon , 95% purity, $10/gallon 99% purity

PBR Catalysts for Carbonylation reaction

(due some research)

<https://www.sciencedirect.com/science/article/pii/S0926860X20300818>

[Links to an external site.](https://www.sciencedirect.com/science/article/pii/S0926860X20300818)

CO : supplied from synthesis gas at a neighboring chemical plant. Has to be purified/separated from H2. $10000/ton.

Heaters/Boilers: can handle any volume you need. Costs $100 and emits 1 ton of CO2 per degreeC-ton of steam/water needed to be heated or boiled.

Chillers/Coolers: can handle any volume you need. Costs $200 and emits 1 ton of CO2 per degreeC-ton of water or alternative coolant to be cooled or chilled

# Environmental & Externalities

Cost of direct CO2 remediation (optional) $80/ton

Cost of indirect CO2 remediation (optional) $50/ton

Cost per mile Acetic Acid sent to market by truck: 1 ton per 500 miles

Cost per mile Acetic Acid sent to market by rail: 1 ton per 1000 miles

Cost per ton of Acetic Acid produced in other environmental contaminants/waste to dispose of

Most ethical / green service: $10000/ton of wastes

Medium ethical / green service: $10000/ton of wastes

Lowest ethical / green service: $10000/ton of wastes

No ethical / green service: $0/ton of wastes, but $3M/ton fines from EPA if caught dumping.

*Chance of getting caught depends on quality of employees hired.*

*3 dumps per week.*

*3 threshhold fines per year = loss of operational license*

*Taxpayers bear cost of cleanup. Taxes increase by 5% on individuals and 10% on corporations if more than 10 tons of waste have to be remediated.*

*Demand for your product is driven by public relations. In the event of a tax increase, your demand will shift the price curve by 30%.*

# Additional Info on General Process for LLE calculations

Based on student requests last evening,

here is a powerpoint and a code workflow idea for doing the LLE part,

IF\* you choose to do it instead of a pure traditional distillation.

These files are attached here and here.

[LLEcodeworkflow.mlx](https://njit.instructure.com/courses/30130/files/5886261?wrap=1)

[Download LLEcodeworkflow.mlx](https://njit.instructure.com/courses/30130/files/5886261/download?download_frd=1)

[LLE-added-info.pptx](https://njit.instructure.com/courses/30130/files/5886267?wrap=1)



[Actions](https://njit.instructure.com/courses/30130/pages/additional-info-on-general-process-for-lle-calculations?module_item_id=1260016#)

NOTE further:

IF you want to take a shortcut approach instead of the above, I will allow it, but you should know it introduces about another 20% error (overprediction of efficiency).

Shortcut approach:

Find the general saturated (maximum concentration) Equilibrium solubility ratio of acetic acid in water vs in kerosone. This will take some literature search to get these values.

Let's say, for example, that Ksmax of acetic acid in water is 0.01, and Ksmax of acetic water in kerosense is 0.02 (note, these are not the ACTUAL values). Ks2/Ks1 = 0.02/0.01=2.

Thus whatever acetic acid comes into the column would fractionate out in a 2:1 ratio assuming you had equal amounts of water and organic solvents streams. (Do the algebra material balance accordingly if the water and organics are not in equal amounts)

If the KS ratio was 3, then it would fractionate out at 3:1 ratio, etc .

**Note, this is a very very crude approximation, but you could chain this together numerically very easily.**

**IF you do this shortcut, assume it overestimates the separation by 20% and account for that accordingly. (The trays are not "ideal").**

**Hope this helps!**

# Other Design Constraints & Regulations

These are basically up to you to think about and add in to your model.

Do you want to follow all OSHA regulations? IF so, let's assume that it costs $ to do so, but you won't have safety incidents.

$500 per day to comply.

Do you not?

$0 per day for compliance, but

$10M in lawsuits and fines for each incident.

Proportionality of incident is 0.01 per day-ton of Acetic Acid produced.

3 Incidents in a month = closure of facility by OSHA

What else would you like to add? Make it YOUR project

Workers' wages?

Worker satisfaction?

State-specific regulations somewhere?

Most energy efficient process regardless of money /etc?

# Further Hints, Tips, and Sample Ideas

general PFR model with cocurrent heat exchange.

[Attached here.](https://njit.instructure.com/courses/30130/files/5843174?wrap=1)

[Download Attached here.](https://njit.instructure.com/courses/30130/files/5843174/download?download_frd=1)

Uses structure in/out appending

Hint/Tip

You might want to use the row feature of your structure variable do represent the piece of equipment in the process.

struct2(1).field1 ...

struct2(1).field2... for properties of the first equipment (a batch reactor for example)

struct2(2).field3.... for properties of the next piece (maybe straight into a distillation).

Remember that you can have empty rows/columns inside a given field. This is allowed!

[Example/demo of this idea above (using structures consecutively)](https://njit.instructure.com/courses/30130/files/5854314?wrap=1)