Learn Aspen Plus in 24 Hours

A proposal for a book and continuing learning community

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Brief Overview

- My Experience:
  - 6 years in teaching process simulations & conceptual process design at undergrad & grad levels
  - Two book chapters:
    - 60 pages on CO_2 capture simulations using Aspen Plus, Aspen Hysys, ProMax, and Pro/II in *Sustainable Reactor Engineering*
    - Contributed to WD Seider's famous book 3rd ed. Chapter was on Aspen Icarus (2006)
- I have developed 12 self-teaching modules (2 hours each)
  - Designed to bring students up to speed in Aspen Plus
  - Suitable for 3rd Year undergraduates and later.
  - Modules are in continual improvement, review, and update
- Materials and concepts been reviewed by faculty and students at:
  - McMaster University
  - West Virginia University
  - Vanderbilt University
  - Northwestern University
  - Auburn University

Introductory Material

Module Objectives in Bullets

Quickly see what is covered in each module

Prerequisite Knowledge

Links to videos, websites, and textbook sections. to get pre-requisite theory knowledge

Reviews knowledge from first 1.5 years of chem. eng. curricula

How can you use this knowledge?

What are the kinds of problems you can solve by using these tools?

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T2 - Physical Properties

Suggested Completion Date: Jan 19, 2016

Chemical Engineering 3G04
Simulation, Modelling, and Problem Solving
Prof. Thomas A. Adams II

Estimated Completion Time

2 hours, plus time required to review past course material to catch up on pre-requisite knowledge.

Objectives

- Utilize the physical property estimation procedures in Aspen Plus for components
- Use the stream analysis tools to estimate stream properties.
- Use theoretical model blocks such as duplicators
- Use a pump to manage pressure differential
- Tweak converge criteria for blocks to overcome convergence problems
- Use distillation models to simulation a pressure swing distillation system
- Construct flowsheets with recycle in an intelligent way by working piece by piece rather than creating one big flowsheet and hitting Run.

Instructions

Complete this tutorial independently. It is worth no credit, so focus on learning the material. Your tutorial time will be set aside for you to work on this tutorial with the help of the TAs or your peers as needed, but you are certainly welcome to work on this in the lab on your own time.

Before you come to lab / getting help

Read this tutorial before coming to lab, if possible. If you do not remember what a distillation column is, it would be helpful to review your separations textbook, as well as this video (and the rest of the distillation section there if that helps) and this website. If you don't know what a pump is, review your fluids textbook, and complete Skills Test 1 available in the Content section of Avenue to Learn. If you do not remember what VLE phase diagrams are, such as Txy and Pxy diagrams, try this video. If you do not know what azeotropes are, try this video. Of course, you should complete all previous tutorials first before attempting this one.

How this material might be assessed

The use of Aspen Plus will be frequently assessed in this course, as mentioned on the previous Tutorial. However, many new concepts that arise in this tutorial might be assessed in a variety of ways. For example, on written exams, I might show you VLE diagrams of binary systems and expect you to use it to help synthesize a process for the separation of the chemicals. For example, you might be required to recognize that there is or isn't an azeotrope, and then determine whether you need to use pressure swing distillation or not. Or, you might need to estimate the distillation and bottoms temperatures, or choose what operating pressure to use for distillation based on a number of factors. Or, I might provide screen captures of VLE tables and ask you to use that information to make predictions about certain process behaviour. You may be asked to sketch out a process which given a feed arrives at a certain set of products at various desired purities, while labeling known quantities or ranges for temperature, pressures, compositions, and/or flows. I may also provide for you stream conditions, results of stream analyses, or pure component analyses and expect you to be able to interpret and use the resulting data to answer questions, such as identifying dew and bubble point temperatures and using that information to make decisions about the flowsheet.

In addition, for the in-lab midterm and the project, you will be expected to be able to use the software in practical ways in order to get at or determine or estimate the information you need to answer questions. For example, you will need to know the actual buttons to push in order to use all of the features and set up the models required. That part may not be explicitly assessed, but rather implicitly as you will need to know what to do in order to even get started. You will also find it necessary to understand convergence, how to tweak the parameters and why, and how to interpret control panel output in order to actually construct and complete simulations at all.

Visuals and Theory

Lots of Screen Captures

ence

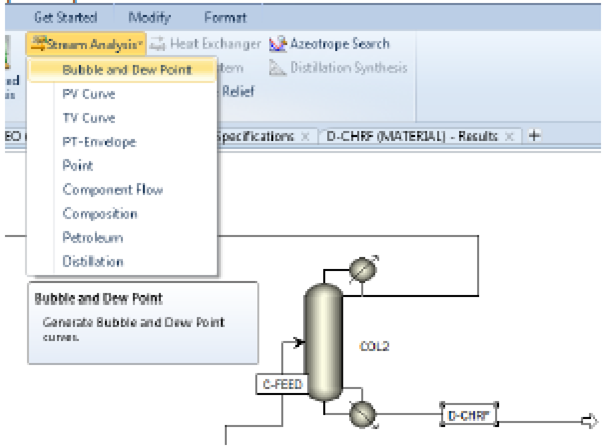
hould be close
.
eotrope (distil-
hould be close

otrope is what
cycle stream to
quick eyeball
8), do not mix
to reduce the
pressure going
atically flash to
e inlet nozzle.

roform?

methanol pro-
predicted but
ed with more
positioning of
another time.

por line intersects is the dew point, and where the liquid line intersects is the bubble point. Similarly, at a constant T, you can find out at the dew and bubble point pressures.



Q12) What is the bubble point temperature in °C of the chloroform product stream at 5.5 bar?

You can get additional information not in the results section, such as viscosity of the mixture (MUMX, MU is "mu" or μ), thermal conductivity (KMX), or surface

Some Theory Covered

Aspen has a lot of physical property data that isn't shown on this form. You can get to it by pressing:

Then head down to the Methods | Parameters | Results tab to see all of the different physical properties or property parameters that in the database. They are all stored in a sort of coded form. For example, "PC" is critical pressure. You could find those out by searching them in the help file.

Look in the T-dependent tab of this form to find out what the equation used for the vapor pressure is (PLXANT-1). Elements 1 through 7 are the coefficients C_1 through C_7 in Antoine's equation:

$$\ln P_i^{sat} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i}\ln T + C_{6i}T^{C_{7i}}$$

Where T is in K.

Q2) What is C_{2i} for i =methane in Antoine's equation as used by the program?

Part 2-Create a VLE Diagram

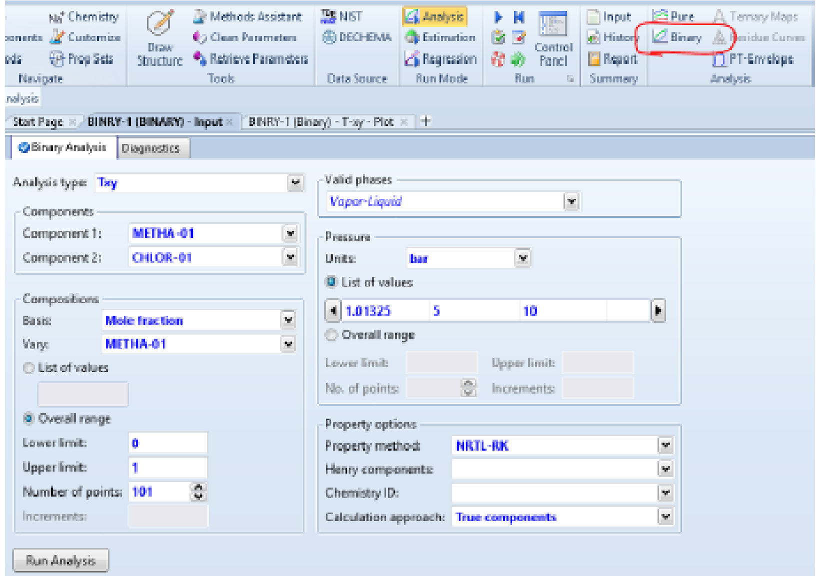
One of the first stages of answering "how do we separate these?" is to look at the vapor-liquid equilibria. This will tell you a lot about how easy it will be to use distillation. Let's first use Aspen to do this.

Aspen Properties has a collection of tools that lets you use the physical property models to make physical property estimations without having to create a flowsheet. Go to the Analysis section of the menu, and then select Binary. This will bring up a little dialog where you can perform equilibria calculations.

To see the VLE it is usually most convenient to see a Txy diagram. Set the analysis type to Txy. You then choose the two components we want to compare (should already be selected by default). You can also select the range of mole/mass fractions of the primary component that you want to look at (usually just leave it at 0 (0% species A, or 100% species B), and 1 (100% species A, and 0% species B)).

You can also tell it how many points to look at. The default is 41 points, which is every 100/(41-1) = 2.5%. Change it to 101 so that we get one data point at every 1 mol %.

In the upper right we can pick which phases we are looking at. Leave it at vapor-liquid for now but note that we can also do vapor-liquid-liquid and special versions of that. See the screen below:



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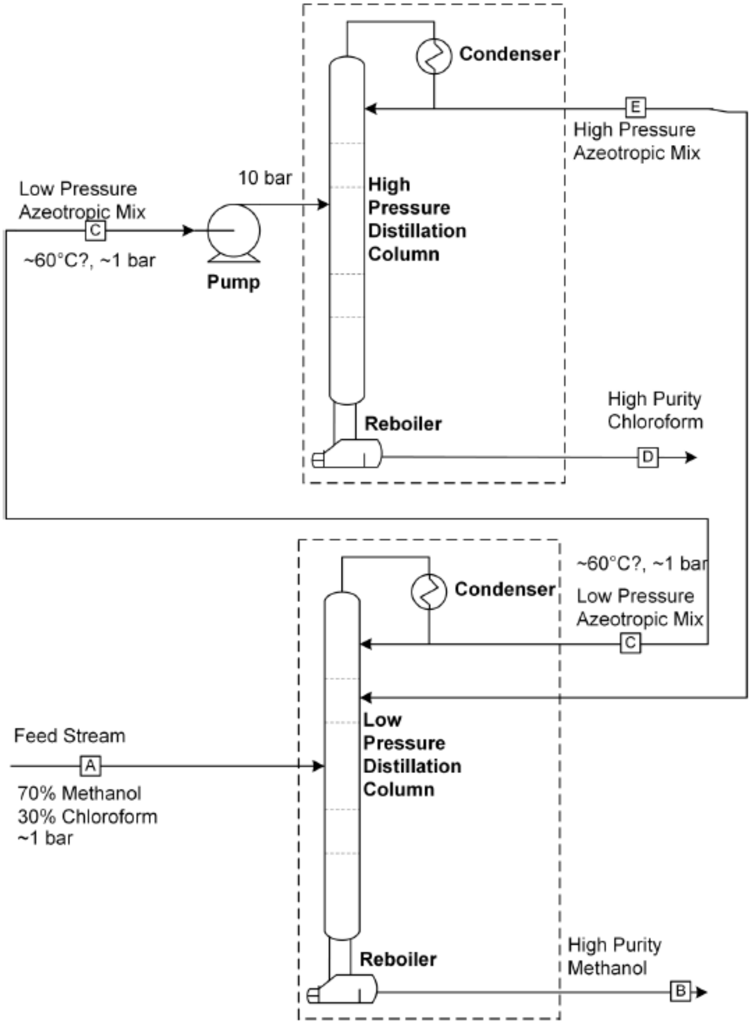
More Examples

Tutorial 2 - Physical Properties & Convergence



8 of 10

Use real flowsheets as examples

Solutions provided visually *(where do I find that number again?)*

ChE 3G04 – Simulation, Modeling, and Problem Solving

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Tutorial 7 Solutions

PART 1

Q1) 1417

	SYNGAS
Temperature C	925
Pressure bar	32
Vapor Frac	1
Mole Flow kmol/hr	1416.8
Mass Flow kg/hr	18341.4
Volume Flow cum/hr	4394.96
Enthalpy Gcal/hr	-32.458
Mole Flow kmol/hr	
METHANE	11.6
WATER	651.6
CO	188.4
H2	565.201

Q2) 224

Q3) 565

	STEAM	SYNGAS-D
Temperature C	237.5	105
Pressure bar	32	32
Vapor Frac	1	1
Mole Flow kmol/hr	223.694	800.486
Mass Flow kg/hr	4029.9	7238.54
Volume Flow cum/hr	261.329	804.69
Enthalpy Gcal/hr	-12.613	-6.774
Mole Flow kmol/hr		
METHANE		11.606
WATER	223.694	35.304
CO		188.394
H2		565.182

Advanced Stuff

should see something like the following (**these numbers are made up, they are not the right numbers!**)

Summary Costs

Item	Material(CAD)	Manpower(CAD)	Manhours
Equipment&Setting	64500.	2596.	112
Piping	26605.	7673.	312
Civil	1530.	1763.	91
Structural Steel	0.	0.	0
Instrumentation	9568.	1706.	64
Electrical	1002.	687.	29
Insulation	0.	0.	0
Paint	1002.	1753.	95
Subtotal	104207	16178	703

al and manpower cost=CAD 120400.

You can see that while the actual pump itself costs $64,500 (CAD), it costs $2,596 to install and required 112 man-hours to do so. Then there is the piping to connect it to the other parts of the plant, instruments such as flow meters, electrical wiring, and paint. The total material and manpower cost, also known as the **total direct cost**, is at the very bottom ($120,400). It is this number that is the most important. It is the number that you'll pay to have this piece of equipment magically appear in your chemical plant. You'll see it also back in the main screen, middle column, by selecting the List tab.

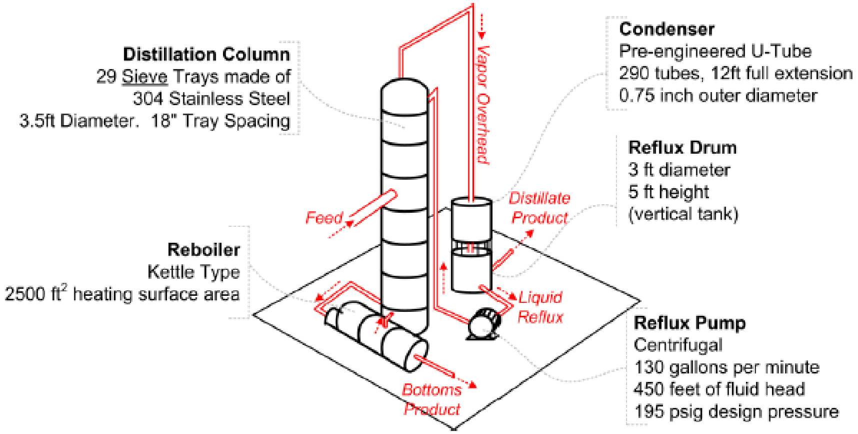
Q1) Report the total direct cost of the reflux pump to the nearest dollar.

Item	User ...	Item Description	Model
1		Reflux Pump	CP CENTRIF

Similarly, add the remaining equipment as shown in the diagram: the condenser, reboiler, reflux drum, and distillation column. Use the specifications given in the figure, and leave anything else at their default values.

- The trayed tower (DTW TRAYED) model should be used for distillation, which includes the trays but does not include the condenser, reboiler, or reflux pump. Change the Application to Distillation with Kettle-type reboiler (DIS-RB).
- For the condenser, you can use a pre-engineered U-tube exchanger (DHE PRE ENGR).
- The reflux drum is a vertical process vessel (DVT CYLINDER). In this case "height" is "tangent to tangent height".
- For the reboiler, use "Kettle type reboiler with floating head" (DRB KETTLE).

Q2) Report the total direct cost of the column (including trays) to the nearest dollar.



Aspen Capital Cost Estimator (formerly Icarus)

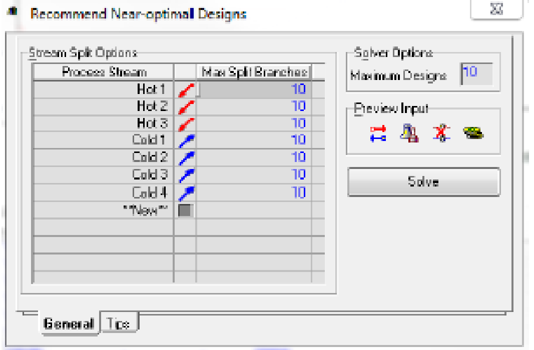
Aspen Energy Analyzer (Heat Exchanger network synthesis)

for the particular process you are working on might be known.

Q3) - What is the number of hours of operation of a plant in a year for a 96 % yearly utilization?

Building the Heat Exchanger Network

The next step is to build the HEN. This means we will try to match process streams to process streams, and process streams to utilities. Click on recommend designs at the bottom of your window. A window pops up titled "Recommend Near-optimal designs".

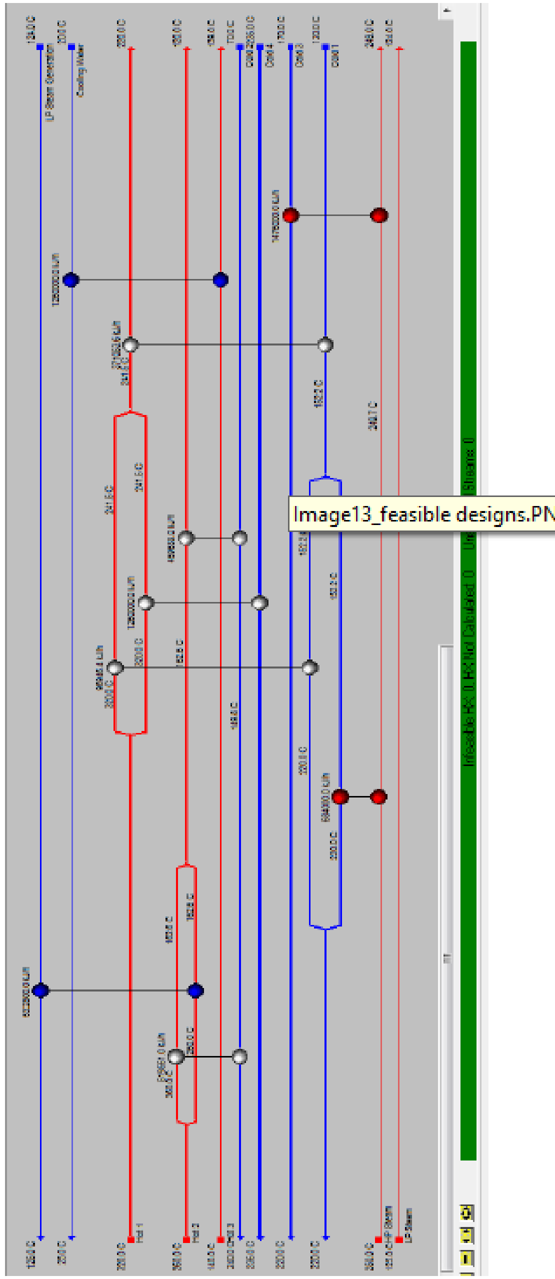


Check to see that in the "stream split options" table the max split branches of all the process streams are at 10. This value can be more or less, but leaving it at 10 allows AEA to have a good number of options for matching streams. Under solver options, type 10 in the box for maximum designs. Again, this value can be more or less but 10 is a good value to choose. Click solve.

The AEA solver runs and generates 10 different designs. If you go through the 10 designs, you will notice the green bars at the bottom of the HEN diagrams.

Green indicates that all heat exchanger matches are feasible, and the heat requirements of all the process streams are satisfied.

Music break

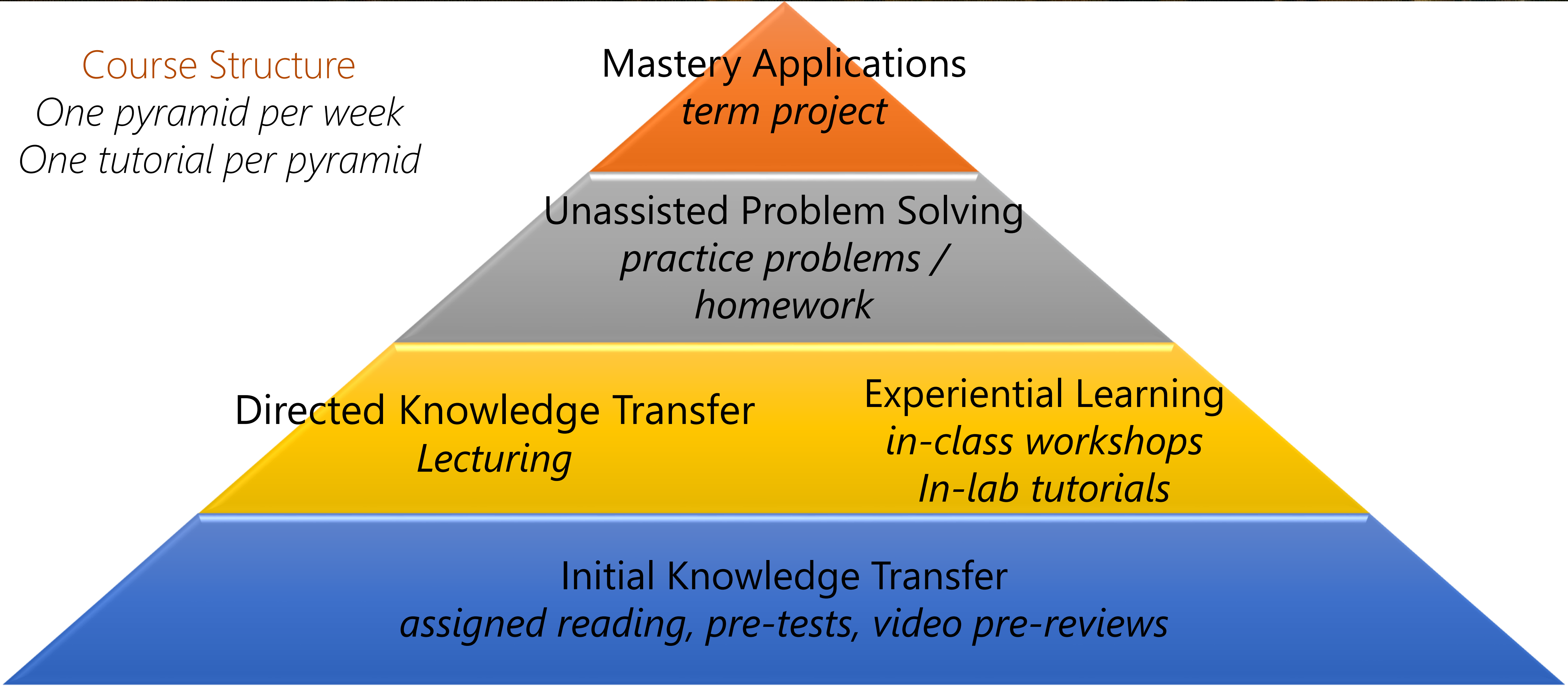


Where They Fit in My Teaching Hierarchy

Course Structure

One pyramid per week

One tutorial per pyramid



Proposed Chapters (Part 1)

1. Getting Started
   - Starting from blank screen
   - Adding chemicals, physical properties
   - Streams and blocks
   - Running simulation
2. Physical Property Modeling
   - Property estimation for components
   - Stream analysis tool
   - Retrieving Parameters from Database
   - Recycle streams
   - Theoretical tools (Duplicators, etc)
3. Problem-solving tools part 1:
   - Sensitivity Analysis
   - Design Specifications
   - Heat & Work streams
4. Problem-solving tools part 2:
   - Utilities
   - Optimization
5. Advanced Reactors Models
   - Batch & Plug flow reactor models
   - Data Fit / Regression for kinetic parameter estimation from data
6. Simple Distillation Models
   - Shortcut distillation (DistWU, Dist)
   - Staged Equilibrium (RadFrac)
   - What if scenarios
   - UNIFAC predictions
   - Property packages and team collaboration

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Proposed Chapters (Part 2)

7. Rate-Based Distillation Models
   - Staged Equilibrium (RadFrac)
   - Strategies for convergence
   - Calculating column diameters, flooding, etc
8. Advancing Modeling Tools
   - Calculator Blocks
   - Custom Models with Fortran
   - Basic Automation with Microsoft Excel
9. Capital Cost Estimator
   - Standalone Product
   - Embedded within Aspen Plus (Economics ribbon)
10. Heat Exchanger Networks
    - Aspen Energy Analyzer
    - Optimal HEN Design
11. Pipeline Models
    - Not fully mature.
12. Life Cycle Analysis with OpenLCA
    - Getting data from Aspen Plus
    - Using the software
    - This may be too far out of scope, but more and more programs need sustainability now.
    - Replace with Solids Tutorial?
    - Replace with built-in CO2 stuff?
    - Replace with Heat Exchanger Module?

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A few notes

- This is meant to be problem solving approach
  - Want students to have the ability to select and use the right tools to solve their problems
  - I don't take a unit based approach. There are other resources for that.

Chemical Engineering Examples Covered

- Alkane Purification
- Azeotropic Pressure Swing Distillation
- Biofuel Purification
- Artificial Flavour Synthesis
- Steam Methane Reforming
- Steam Power Plants
- Nuclear Power Systems
- Hydrogen Production
- Methanol production
- Gas-to-liquids
- Dividing Wall Columns

Feedback from Peer Reviewers

- Scott Guelcher (Vanderbilt)
  - Reviewed by design faculty
  - Positive reviews
  - Would use it in 4^{th} semester computational course (2^{nd} year?)
    - 3 weeks introducing students to the material, starting from a blank screen
  - They would like to have the modules be fully independent
    - could be used *ad hoc* in any course as it is needed, starting with 2^{nd} year course.
- Mario Eden (Auburn)
  - Suggested online community
    - Book evolves over time with contribution by others
    - The Perry's of PSE software
- Fernando Lima (West Virginia)
  - Reviewed by undergrads there
  - Enjoyed the material, thought it was appropriate (4^{th} year / senior student)
  - Noted that there are references to other courses / ideas that are not in the course material
    - Needs to be generalized somewhat.
- Fengqi You (Cornell)
  - "Everything looks good to us. We did not observe any issue"

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Proposed Framework

- Book / e-book created and distributed
  - Need to pick publisher, distribution model.
  - Price? Student support material, should not be too large.
- Website created to support book
  - Center for discussion and feedback
  - Discussion Board
- Professors can:
  - Assign book as a course text
  - Cherry-pick individual modules to use in course packs, etc.
- LONG TERM:
  - I become editor of book with multiple contributors / authors
  - Other people and I can add modules, improvements
  - Partially finished modules
    - Aspen Custom Modeller
    - Solids Handling
  - Extremely Useful Additions:
    - Troubleshooting hard-to-converge blocks and loops (especially absorption)
    - External automation
    - External optimization
    - Parallel computing
  - Continuously develops, updates, and improves over time.

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Progress So Far

- Grad Student TA (Trevor West) led new trial with 120 undergraduate students using it Spring term 2016
  - Gathered informal undergrad feedback
  - Made improvements to wording and explanations
- Former Student (Dr. Jaffer Ghouse) has been updating the original tutorials to reflect Aspen v9.
  - About half way done.
  - May end up as second author in the long term.
- Still need to neuter the material for book form.

Proposed Timeline

Update screen captures and text for v9.0
- November - January

Submit proposal to publisher
- December 2016

Revise Chapters 1-3 for Book Format
- December 2016

Chapters 4-6
- January 2017

Chapters 7-9
- February 2017

Chapter 10-12
- April 2017 (need more time for one chapter)

Submit manuscript draft to editors
- May 2017

Construct CAChE website for support material
- May 2017
- Include solutions files with professor login?
- Would include my class slides which go with those topics?

Final manuscript edits submitted
- June 2017

PDF version published! Softcover likely later.
- August 2017
- Early proof version can be made available to subscribers.

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