

Learn Aspen Plus in 24 Hours

Integrating Aspen Plus into the Chemical Engineering Classroom



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About Us: Tom

- Associate Professor, **McMaster University**
- **Research**: Chemical process design, modelling, and simulation
- **Education**:
 - B.S. Chemical Engineering (**Michigan State**)
 - B.S. Computer Science (**Michigan State**)
 - PhD Chemical and Biomolecular Engineering (**UPenn**, Warren D. Seider)
- Key Relevant Course Taught:
 - **Process Modelling and Simulation**
 - 3rd Year Course
 - "Pre-Design"
- Aspen Plus user **since 1999**.



About Us: Mario

- Professor and Chair, **Auburn University**
- **Research:** Chemical process/product synthesis/design
- **Education:**
 - M.S. Chemical Engineering (**Technical University of Denmark, DTU**)
 - Ph.D. Chemical Engineering (**DTU**, Rafiqul Gani)
- Key Relevant Course Taught:
 - **Process Synthesis, Simulation, and Optimization**
 - **Process Design Practice**
 - 4th Year Courses,
 - Two Course Capstone Design Sequence
- Aspen Plus user **since 2001**.



Today's Workshop

1. Introduction to Aspen Plus
2. Overview of the *book Learn Aspen Plus in 24 Hours*
3. Workshop 1 – Use Aspen Plus!
4. Using in undergrad courses:
 1. Design Courses
 2. Pre-design or flowsheeting courses
 3. Piecemeal through degree program
5. Experiential learning and working with students in the labs
6. Using for graduate education
7. Workshop 2 – More hands on
8. How to get help?
9. Accessing resources

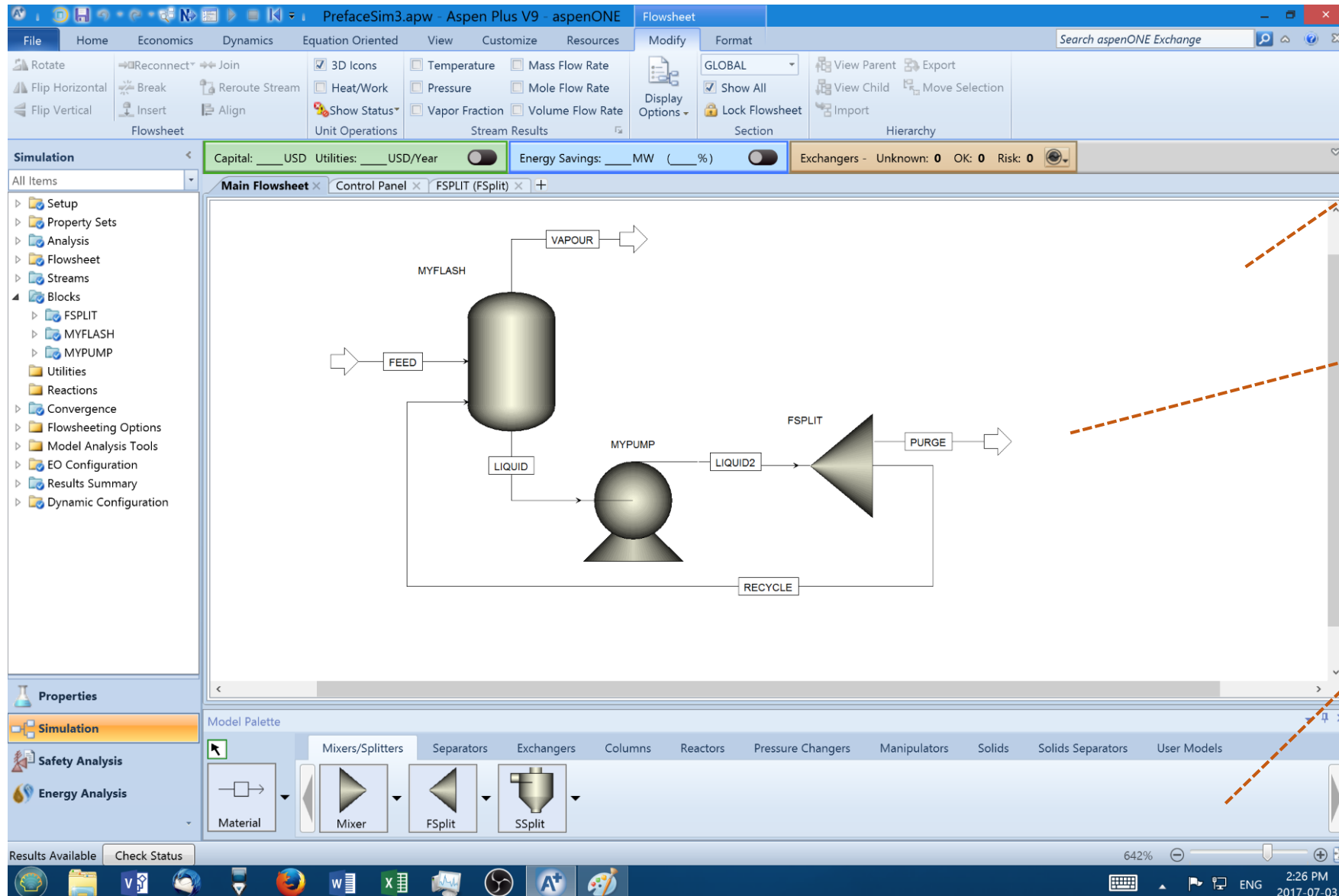


jfr photography

1. Introduction to Aspen Plus

Steady State Chemical Process Modelling

Chemical Process Flowsheet Simulator



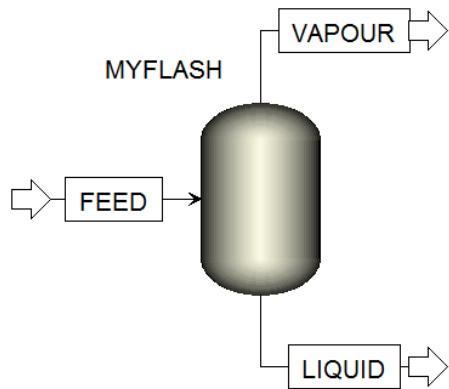
The main flowsheet consists of **streams** and **blocks**

Users build flowsheets through a **visual interface**

A library contains **models** for many different kinds of **chemical process units**

Simple Example: A Flash Drum (steady state)

Users enter known stream data and model parameters into forms.



The screenshot shows the Aspen Plus software interface. The 'Main Flowsheet' tab is active, displaying the 'FEED (MATERIAL)' stream and the 'MYFLASH (Flash2)' unit. The 'Specifications' tab for the flash drum is open, showing the following settings:

- Flash Type: Temperature Pressure
- State variables:
 - Temperature: 50 C
 - Pressure: 1.2 bar
 - Vapor fraction: (empty)
 - Total flow basis: Mole
 - Total flow rate: 100 kmol/hr
 - Solvent: (empty)
- Reference Temperature:
 - Volume flow reference temperature: C
 - Component concentration reference temperature: C
- Composition table:

Component	Value
WATER	50
METHAN...	50
Total	

The 'Valid phases' dropdown is set to 'Vapor-Liquid'.

This flash drum model contains equations for:

- Mass Balances
- Energy Balances
- Fugacity Balances
- Pressure Drop

The physical properties database contains data and correlations for:

- Physical properties of chemicals
- Binary VLE Models

Example Solution

Main Flowsheet x FEED (MATERIAL) x Control Panel x +

▶ ▶ ■ 🔍 Clear Messages Check Status Run Settings

<< All Blocks Reinitialized >>

<< Run reinitialized 14:49:28 Mon Jul 3, 2017>>

->Processing input specifications ...

Flowsheet Analysis :

COMPUTATION ORDER FOR THE FLOWSHEET:
MYFLASH

->Calculations begin ...

Block: MYFLASH Model: FLASH2

->Simulation calculations completed ...

*** No Warnings were issued during Input Translation ***

*** No Errors or Warnings were issued during Simulation ***

Show Sequence

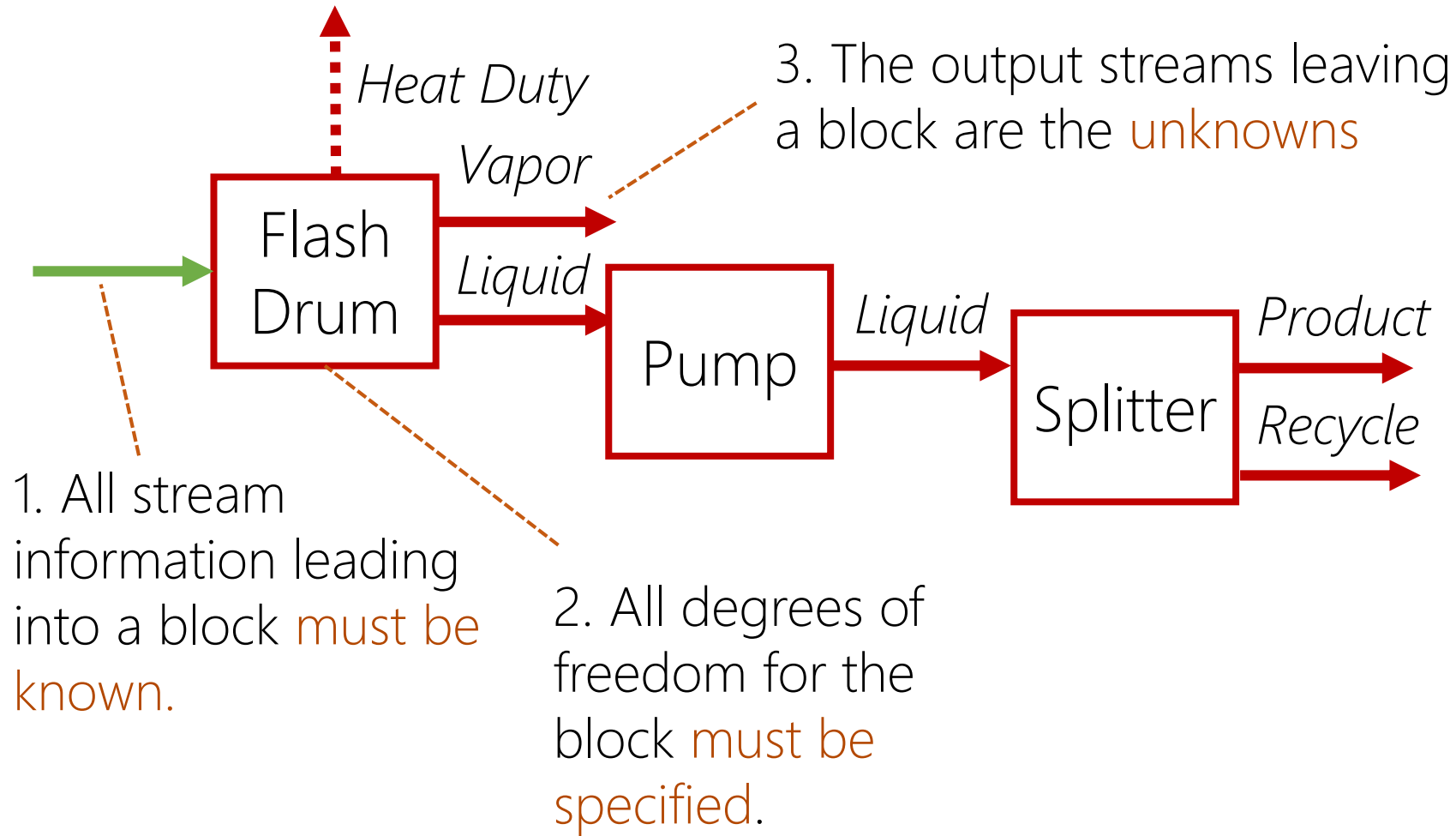
Show EO Control

LIQUID (MATERIAL) - Results (Default) x +

Material Vol.% Curves Wt. % Curves Petroleum Polymers Solids ☒ Status

	Units	LIQUID ▾	VAPOUR ▾
▶ Mass Vapor Fraction		0	1
▶ Mass Liquid Fraction		1	0
▶ Mass Solid Fraction		0	0
▶ Molar Enthalpy	cal/mol	-64527.6	-51216.8
▶ Mass Enthalpy	cal/gm	-3007.83	-1920.23
▶ Molar Entropy	cal/mol-K	-39.6998	-20.1928
▶ Mass Entropy	cal/gm-K	-1.85053	-0.757072
▶ Molar Density	mol/cc	0.030611	3.45199e-05
▶ Mass Density	gm/cc	0.656705	0.000920721
▶ Enthalpy Flow	cal/sec	-564446	-974677
▶ Average MW		21.4532	26.6722
▶ - Mole Flows	kmol/hr	31.4905	68.5095
▶ WATER	kmol/hr	23.7723	26.2277
▶ METHANOL	kmol/hr	7.71821	42.2818
▶ + Mole Fractions			
▶ + Mass Flows	kg/hr	675.572	1827.3

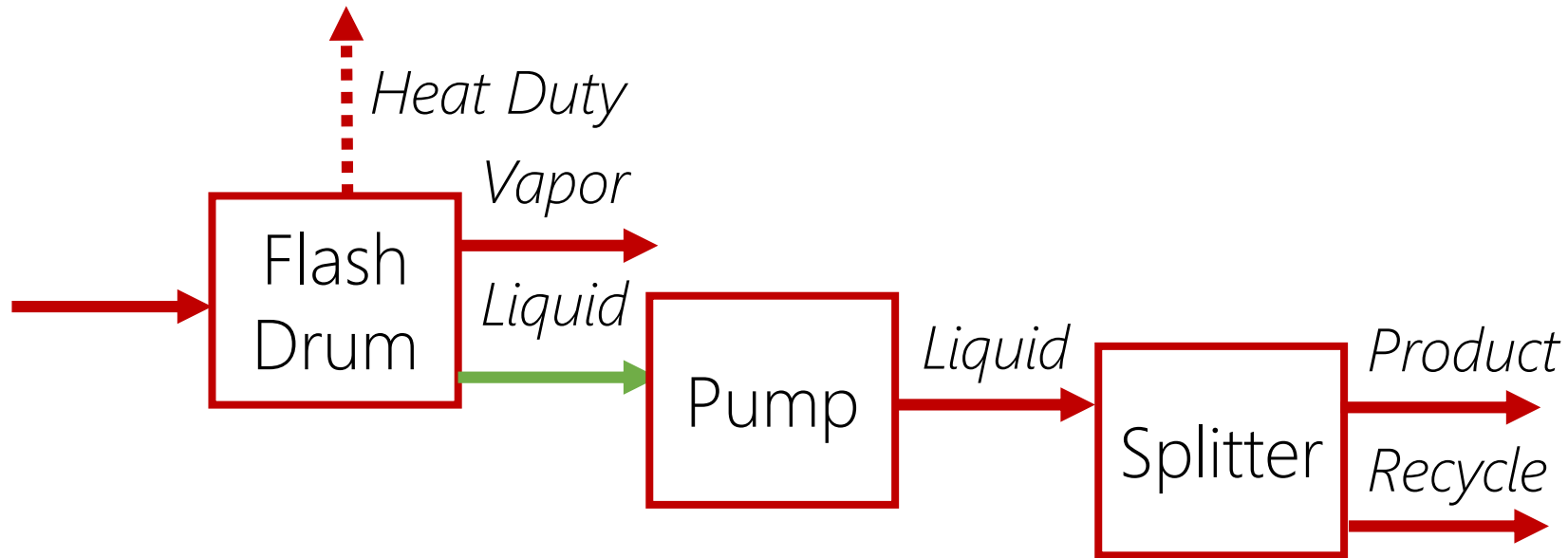
Sequential Modular Flowsheeting



When the simulation is executed, the flowsheet solver **looks for blocks that have enough input information** to solve.

Then a **model-specific subroutine** is run in order to compute the steady-state outputs. It **does not use a general equation solver** (by default).

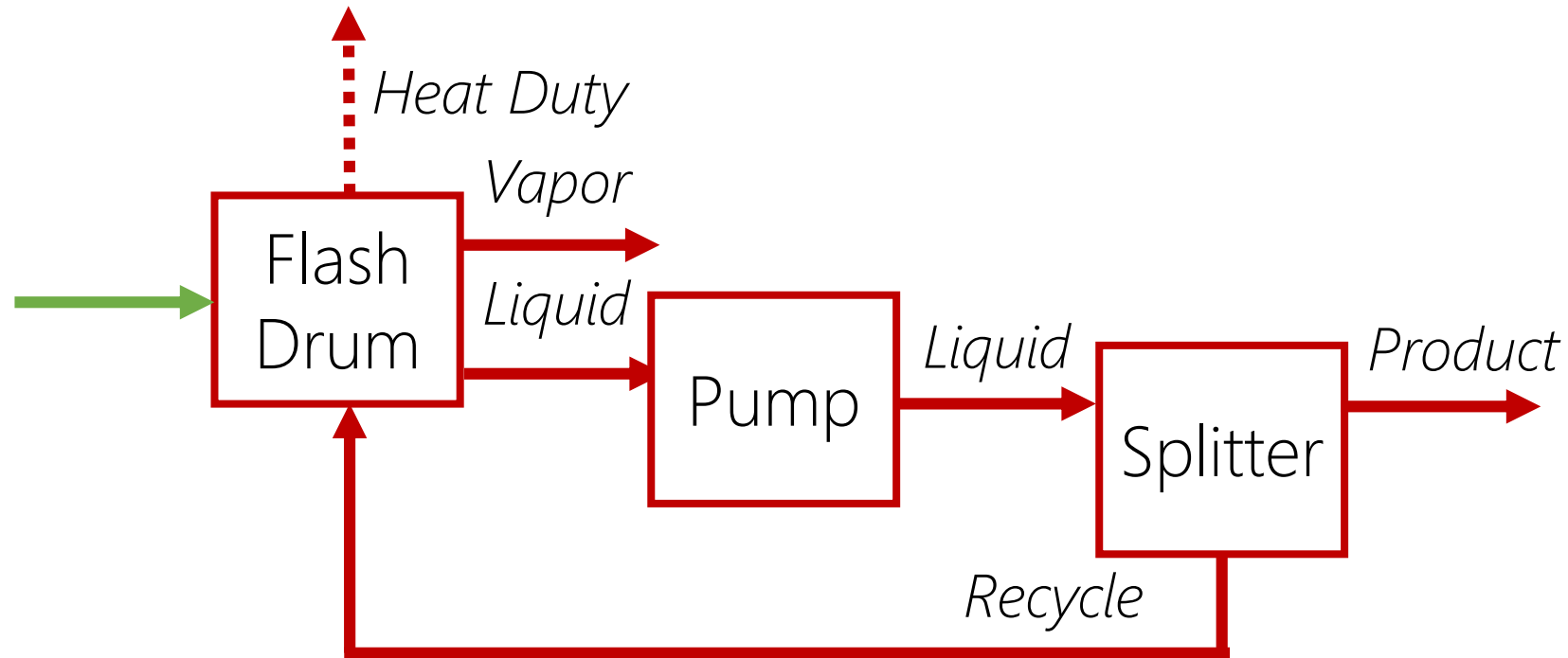
Sequential Modular Flowsheeting (2)



What if we know what we want downstream but we don't know the feed conditions or block settings to get it?

Special tools for that. Sophisticated guess-and-check.

Sequential Modular Flowsheeting (3)

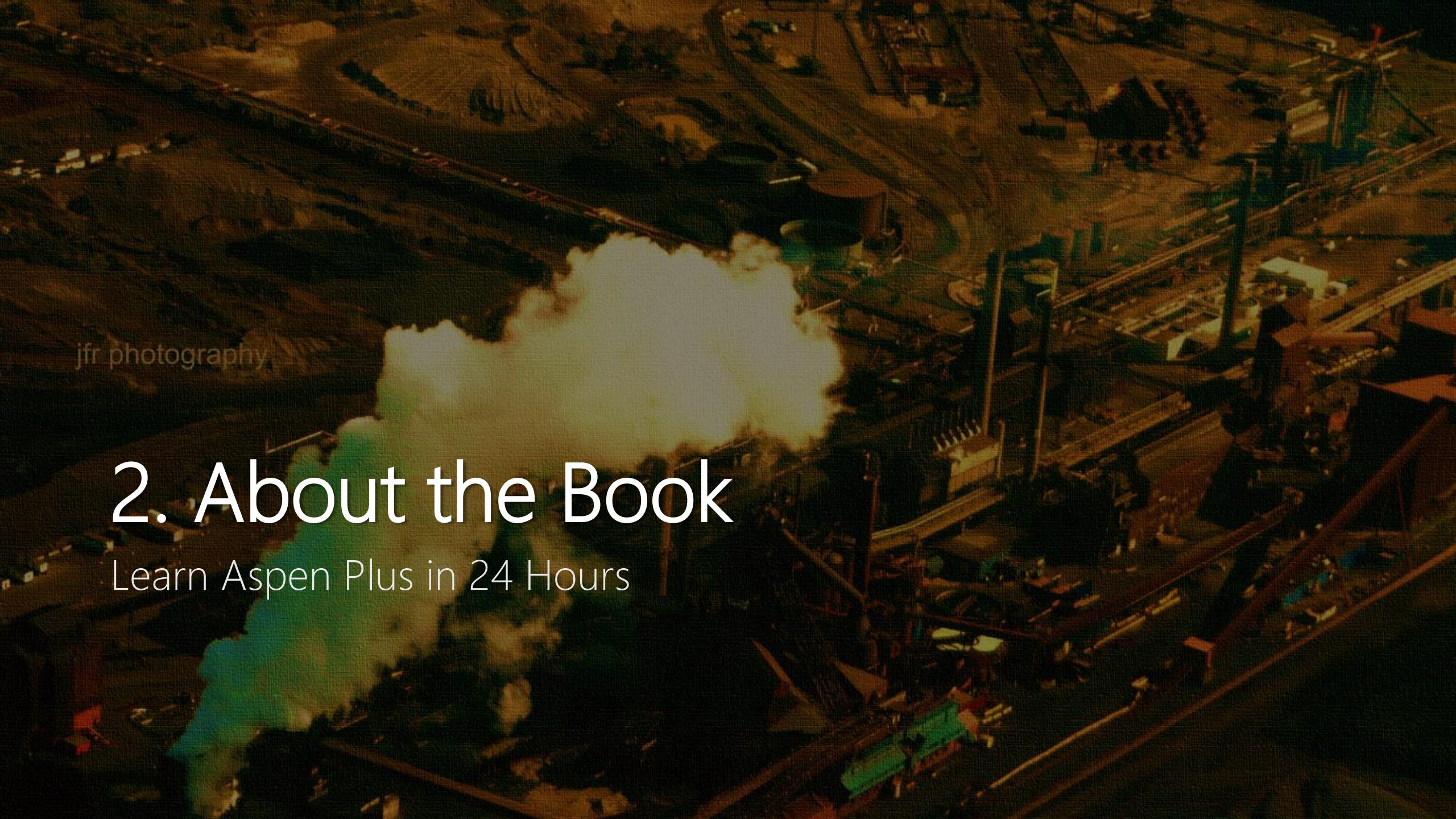


What if there is recycle?

Special tools for that too. More sophisticated guess-and-check.

Aspen Plus vs. Other Competing Software

Our ratings, as appropriate for an undergraduate course setting	Aspen Plus	Aspen HYSYS	Pro/II	ProMax	gProms	COCO
Cost of academic licenses	Free*	Free*	Free	Free*	Low	Free
Installation on student computers	No	No	No	?	?	Yes
Extensive property / chemicals database	Best	Best	Good	Ok	Ok	Poor
Extensive unit operation models	Best	Best	Good	Ok	Good	Poor
Commercially relevant	Yes	Yes	Yes	Yes	Yes	Limited
Ease of use, Ease of Teaching	Not Easy	Not Easy	Easier	Easier	Hard	Ok
Connectivity with Microsoft Excel	Yes	Yes	Yes	Yes	Yes	Yes
Capital cost estimation	Yes	Yes	No	No	No	No
Heat exchanger network optimization	Yes	Yes	No	No	No	No
Extendible to dynamic simulation	Good	Best	Good	No	Best	No
Market Share / Popularity	Most	Good	Good	Some	Good	Little

An aerial photograph of a large industrial complex, possibly a refinery or chemical plant. The facility is composed of numerous interconnected pipes, storage tanks, and structural steel frameworks. A massive, billowing plume of white smoke or steam rises from the central part of the complex, partially obscuring some of the structures. The surrounding landscape appears to be a mix of industrial infrastructure and some open ground. The overall tone of the image is somewhat dark and industrial.

jfr photography

2. About the Book

Learn Aspen Plus in 24 Hours

Learn Aspen Plus in 24 Hours

- Textbook development partially funded by Computer Aids for Chemical Engineering Corporation (CACHÉ Corp).
- Twelve 2-Hour Tutorials
- Based on computer lab modules developed at McMaster University
 - Seven years of development
 - Student and instructor feedback from multiple universities
- Will be a part of a continuously updated online community.

THOMAS A. ADAMS II

LEARN ASPEN PLUS®
IN 24 HOURS



Table of Contents

Preface	
1. Getting Started	<i>Starting from a blank screen with no prior knowledge</i>
2. Physical Property Modeling	<i>Choosing physical properties. Understanding the database.</i>
3. Problem Solving Tools	<i>Design Specs and Sensitivity Analyses</i>
4. Heat Exchangers	<i>HEATER, HEATX</i>
5. Advanced Problem Solving Tools	<i>Utilities, GHG Emissions, Optimization</i>
6. Chemical Reactor Models	<i>RSTOIC, REQUIL, RYIELD, RGIBBS, RCSTR, RPFR</i>
7. Equilibrium-based Distillation Models	<i>RadFrac (in equilibrium mode)</i>
8. Rate-based Distillation Models	<i>RadFrac (in rate-based mode)</i>
9. Custom Models and External Control	<i>USER Blocks (Fortran Code), Microsoft Excel Connectivity</i>
10. Capital Cost Estimation	<i>Aspen Capital Cost Estimator</i>
11. Optimal Heat Exchanger Networks	<i>Aspen Energy Analyzer</i>
12. Solids Processing and Electrolyte Chemistry	<i>Basic solids modelling. ElecNRTL. True vs Apparent components</i>
Solutions	
Command Index	

Chemical Engineering Examples Covered

- Alkane Purification
- Azeotropic Pressure Swing Distillation
- Biofuel Purification
- Artificial Flavor Synthesis
- Steam Methane Reforming
- Steam Power Plants
- Nuclear Power Systems
- Hydrogen Production
- Methanol Production
- Chemical Looping
- Dividing Wall Columns

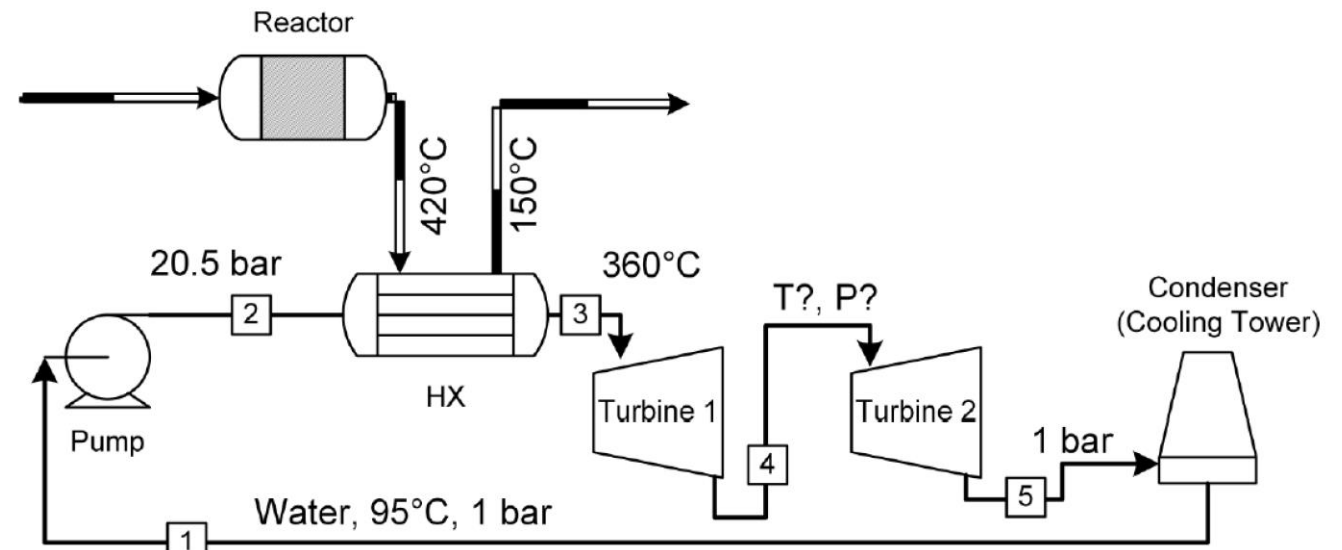


Figure 3.1 A process to generate electricity by using heat from a reactor.

Introductory Material

Tutorial 5

Module Objectives in Bullets
Quickly see what is covered
in each module

Prerequisite Knowledge

Links to videos and websites 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?

Advanced Problem Solving Tools

Objectives

- Learn to use the Utilities feature in Aspen Plus
- Use simulations to compute utility costs
- Learn the Optimization feature in Aspen Plus
- Combine the two features to design a process to have the lowest energy costs

Prerequisite Knowledge

It is advisable to complete all prior tutorials before you begin this one. At this point, you'll need to understand distillation, valves, pumps, and VLE diagrams. If you still don't understand distillation, I suggest you try watching the four videos in the distillation section of the LearnChemE website.¹ You will also need to have a basic understanding of the first and second laws of thermodynamics as they relate to heat transfer (specifically, the basic concepts of energy balances and that heat cannot transfer from cold to hot spontaneously) as these concepts are very important for the selection of utilities. You may also be interested in a short video introducing the concept of optimization.²

Why This Is Useful for Problem Solving

The Utility feature in Aspen Plus is incredibly useful for design projects, because it can be applied so many times, and it makes it much easier to determine and optimize process costs when used in the correct fashion. To reduce the utility costs of a process you will need to know what types of utilities (such as steam, fired heat, cooling water, and refrigeration) are available, their operating conditions (i.e., temperature and pressure),

¹<http://www.learncheme.com/screencasts/separations-mass-transfer>. This is peer-reviewed material produced by the University of Colorado, Boulder.

²<https://www.youtube.com/watch?v=YSewtL3tYY>. This is a video from the AIChE Academy.

Visuals: Over 240 Screen Captures and Figures

Flowsheets

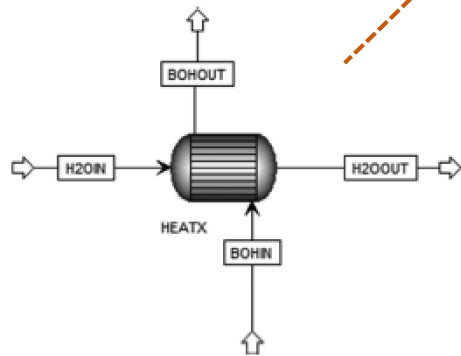


Figure 4.11 A model of the same heat exchanger, but using a single HeatX block.

After selecting Shortcut as the Model fidelity choose Countercurrent as the Shortcut flow direction and Design as the Calculation mode. Under the Specification drop-down we have different options from which to choose. Since we know the outlet temperature of butanol we want, select Hot stream outlet temperature, and enter 40°C as its value. Furthermore, enter 10°C as the minimum temperature approach (ΔT_{min}), as shown in Figure 4.12. Assume that there is no pressure drop in the heat exchanger, and leave the heat transfer coefficient (in the U Methods tab) at the default.

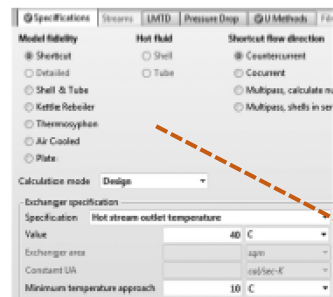


Figure 4.12 Directly specifying the temperature approach in a HeatX model.

TUTORIAL 43

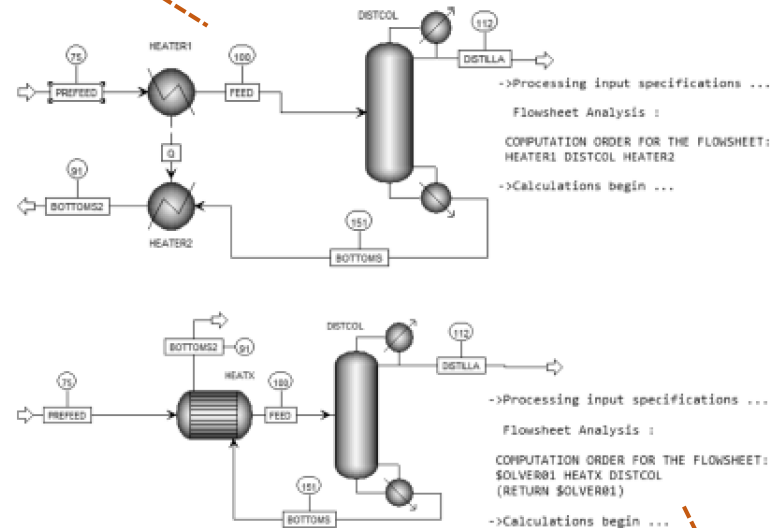


Figure 4.17 Two different models of the same process that uses an economizer integrated with a distillation column.

getting distillation column models to work can be very difficult or time consuming, and so knowing how to use the two Heater approach may be critical to get certain stubborn flowsheets to converge quickly and reliably. However, if a HeatX works to your satisfaction, just use it.

Music break

Understanding Program Output

20 PHYSICAL PROPERTY MODELING

Basically, what has happened is that the simulation model did not successfully get a result. Why not? The Fortran routine which solves the RadFrac block uses an iterative guess-and-check procedure, and after 25 guesses it did not find a solution (did not converge). However, the Err/Tol number tells us how close it is to converging.

This error of the simulation is the norm of all model equation residuals. The residuals are the left-hand sides of the equations minus the right-hand sides of the equations. The tolerance is the maximum amount of error that is allowed. So if Err/tol is above 1, then we're not done converging because some of the equations have too much error, so not all of the variables have been solved to our satisfaction. If Err/tol is below 1, then we have solved the problem within tolerances. The point is that if it is heading toward 1, we are on the right track. It can be a bit of an art form to look at a sequence of Err/Tol numbers and decide whether the solver is approaching a solution, or it is going nowhere. A good rule of thumb is that the Err/Tol is staying below 1000 and has not recently risen above 100,000 then it is probably on the right track.

So, let's tell the program to keep trying. To do this, go to Blocks | Column Name | Convergence, (or double-click on the column to get to Blocks | Column). Under Basic, you will see that "maximum iterations" is at 25 by default. Change it to 200 (the maximum), as shown in Figure 2.9. Rerun the simulation. It should converge now.

OL	ML	IL	Err/Tol
1	1	10	1294.1
2	1	9	2880.4
3	1	7	2323.0
4	1	5	1368.4
5	1	5	782.19
6	1	5	603.68
7	1	4	234.89
8	1	3	89.374
9	1	3	74.645
10	1	4	87.531
11	1	4	201.01
12	1	5	1168.0
13	1	3	377.31
14	1	3	378.22
15	1	4	458.58
16	1	4	389.38
17	1	8	922.52
18	1	6	1907.1
19	1	10	1970.3
20	1	7	675.34
21	1	8	687.84
22	1	7	914.43
23	1	5	475.38
24	1	3	380.79
25	1	5	339.36

Figure 2.8 Control panel output for a RadFrac simulation that did not converge, and so the model outputs were not computed satisfactorily.

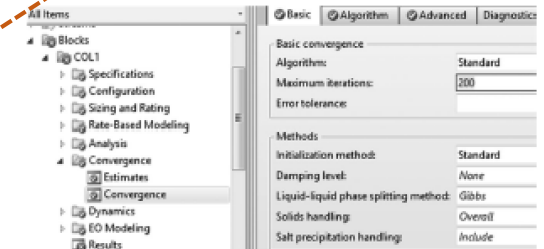


Figure 2.9 The Convergence form for the RadFrac block. Use this to change the maximum iterations and other parameters of the underlying numerical methods used to solve the model equations.

³Recommended listening: *Take a Chance On Me* by Abba.

Theory and Problem Solving

Solutions are provided visually

TUTORIAL 13

What has happened is that we now need to add the binary interaction parameters between methanol and chloroform. The NRTL part of the NRTL-RK model is an activity-coefficient based model which is used to predict liquid-phase activity coefficients γ_i as a function of temperature and composition. I am sure you remember activity coefficients? They form the basis for writing *fugacity balances*. Yeah, I just went there.⁷

At vapor-liquid equilibrium, the fugacity of each component i in the liquid phase equals the fugacity of each component i in the vapor phase.

$$f_i^L = f_i^V$$

So let's say I have a mixture of water and ethanol at vapor-liquid equilibrium. The fugacity of water in both the liquid and vapor phase might be 6.5 bar, and the fugacity of ethanol in both the liquid and vapor phase might be 2.5 bar. I made up those numbers, but you get the idea.

An activity-coefficient model like NRTL, lets you compute *liquid-phase* fugacities like this:

$$f_i^L = x_i P_i^{\text{sat}} \gamma_i$$

Where x_i is the liquid-mole fraction, P_i^{sat} is the saturation pressure (a.k.a. vapor pressure), and γ_i is the activity coefficient of i . The vapor pressure is a known function of temperature (e.g., you could use Antoine's equation).

The activity coefficients are also a function of temperature and composition. The model that NRTL uses in particular to compute this is as follows:

$$\ln \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ji}}{\sum_k x_k G_{ki}} \left(\tau_{ji} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right)$$

where

$$\tau_{ij} = A_{ij} + B_{ij} T^{-1} + E_{ij} \ln(T) + F_{ij} T \quad \forall i \neq j$$

$$\tau_{ii} = 0 \quad \forall i = j$$

$$G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$$

$$\alpha_{ij} = C_{ij} + D_{ij} (T - 273.15 K)$$

Ok, that's a lot to handle. For now, just worry about this: the terms A_{ij} through F_{ij} are *constants* that are determined by regression of experimental data. They are the same for each pair of chemicals at any temperature, pressure, or composition. They are just fixed numbers and Aspen Properties has a nice database containing thousands of these constants for many different pairings of chemicals. To load them, click on the red

⁷Oh Dr. Adams, that's the evilest thing I can imagine!

Real chemical engineering problems

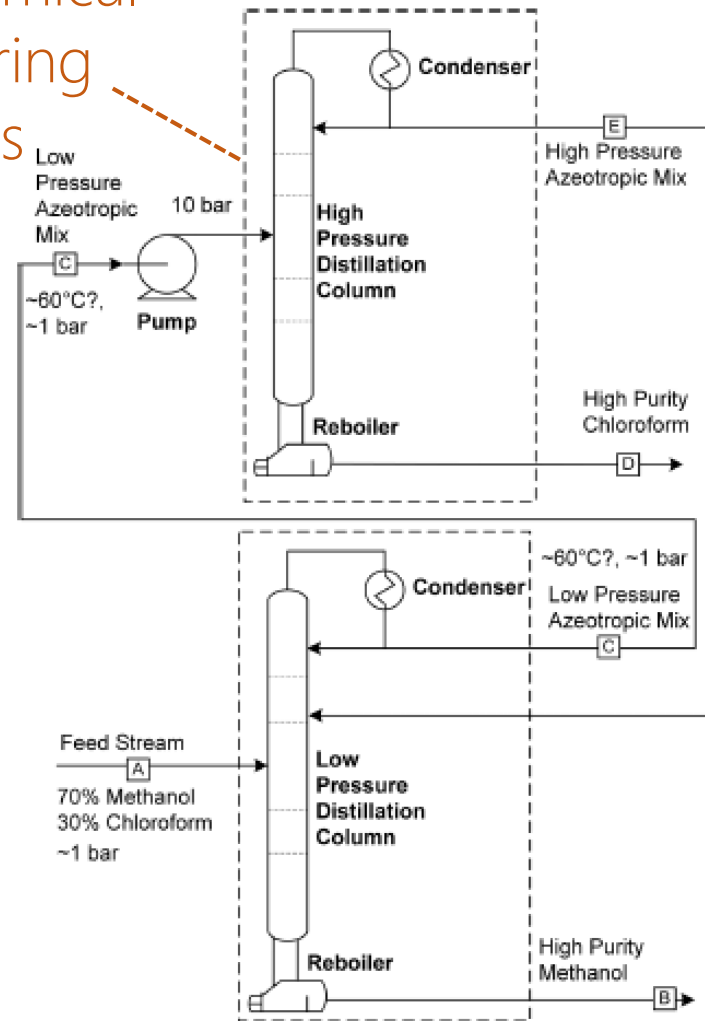


Figure 2.7 The final process as designed by using the Txy diagrams as a guide.

Tutorial 7 Solutions

PART 1
Q1) 1417

	SYNGAS
Temperature C	925
Pressure bar	32
Vapor Frac	1
Mole Flow kmol/hr	1415.8
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

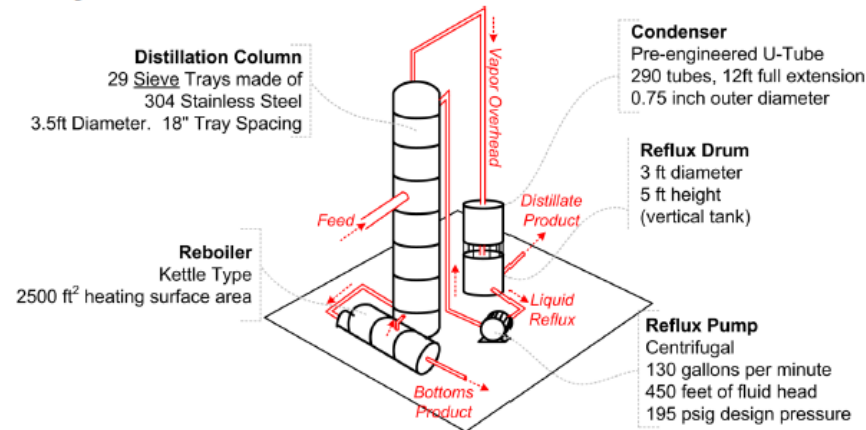
Tutorial 8 - Capital Cost Estimates with Aspen Capital Cost Estimator

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	1510.	1763	91
Structural Steel	0.	0.	0
Instrumentation	9568.	1706	64
Electrical	1002.	687.	29
Insulation	0.	0.	0
Paint	1002.	1753	95
Subtotal	104287	14178	783

al and manpower cost=CAD 128400.

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)

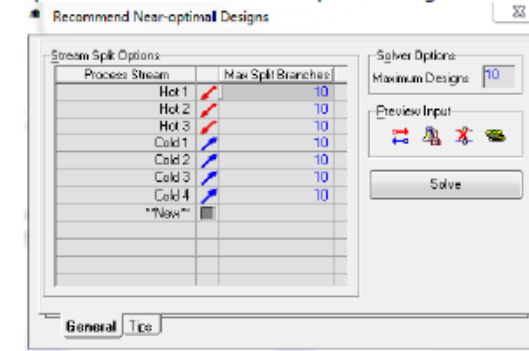
Tutorial 9 - Heat Exchanger Networks

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

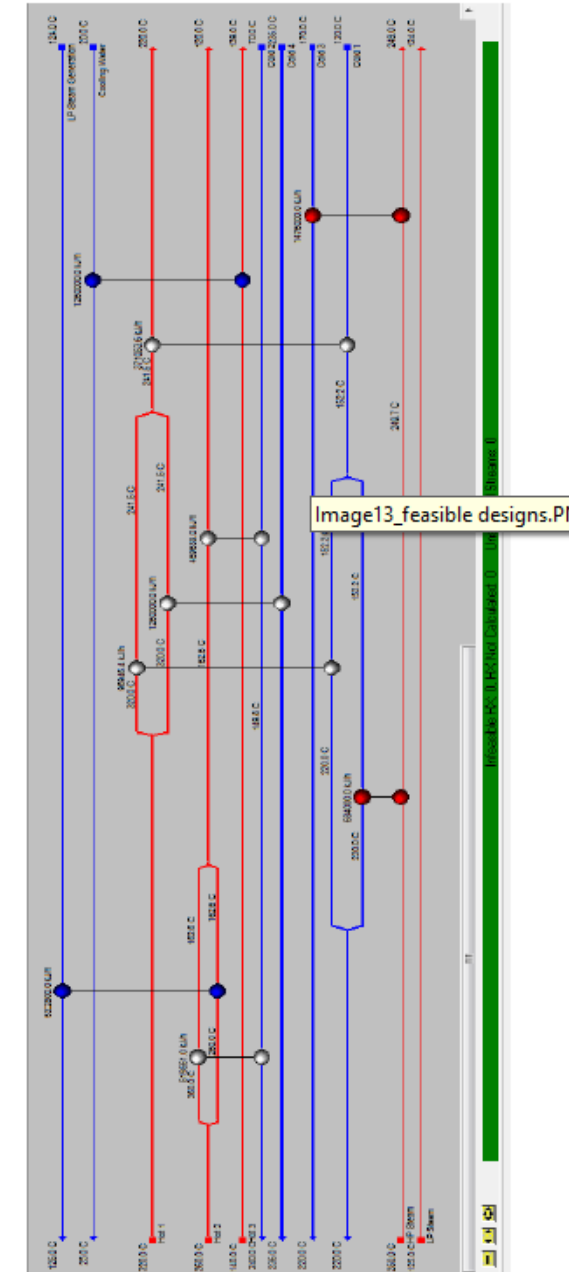
The next step is to build the HEN. This means we will try to match process streams to process streams, and process streams to utilities. Click on recommend designs at the bottom of your window. A window pops up titled "Recommend Near-optimal designs".



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



jfr photography

3. Workshop 1

Time to try it!

- Novice Users, try Tutorial 1
- Experienced users, try Tutorial 5
- We'll come around the room, help and answer questions.

An aerial photograph of a large industrial complex, possibly a refinery or chemical plant. The facility is characterized by a dense network of pipes, walkways, and various industrial structures. In the center-left of the image, a massive, billowing plume of white smoke or steam rises high into the air, partially obscuring the structures beneath it. The overall color palette is dominated by the greys and browns of the industrial equipment, with the bright white of the smoke providing a stark contrast. The lighting appears to be from a low angle, casting long shadows and highlighting the textures of the smoke and the ground.

jfr photography

4. Using in Undergraduate Courses

Integrating into Year Long Courses

- **Example:** Design or Pre-Design courses.
- **Recommended Use:** One 2-hour computer lab session per week
 - 1 competent instructor/TA **per 20-25** students is enough, more is better
 - **Pick and choose tutorials** that coordinate with your schedule
 - Tutorial 1 can actually happen before first day of lecture!
 - **Students should work individually**, but ok to talk to neighbors
- **Lecture Complement:**
 - **Not Recommended:** Using lecture time to prepare students for the tutorial
 - **Recommended:** Using lecture time to go into more detail and depth
 - **Example for unit ops / design:** The models under the hood of each block and how they link to real equipment.
 - **Example for modelling course:** Sequential modular flowsheeting, algorithms, etc.

Where They Fit in My Teaching Hierarchy

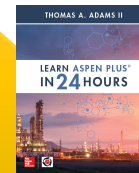
Course Structure
One pyramid per week
One tutorial per pyramid

Mastery Applications
term project

Unassisted Problem Solving
practice problems /
homework

Directed Knowledge Transfer
Lecturing

Experiential Learning
in-class workshops
In-lab tutorials



Initial Knowledge Transfer
assigned reading, pre-tests, video pre-reviews

Tutorial Assessment Strategies

Strategy	Disadvantages	Advantages
Requiring students to answer the questions in the text and having them graded	- Someone has to grade it - Auto-grading is too unforgiving <u>Student feedback:</u> - Created high anxiety situation - Students not focusing on digesting the material, only trying to get the points	- An "Easy" way to earn points. ... all the answers are now in the back of the book, sorry...
Writing your own questions that change from year to year (Example, changing flows, temperatures, etc)	- All of the above, plus: - Someone has to change it every year.	- An "Easy" way to earn points. - Year-to-year answer copying not possible
No assessment—tutorials are purely optional	- In-lab attendance was very poor - Overall learning was very poor	- Easy on the instructor - Low anxiety for the students
No assessment—points for attendance worth small amount of total course grade	- Bottom 5-10% of students did not finish the material within two hours - Some students wanted to be assessed	- Easy on the instructor - Low anxiety for the students - Student learning was excellent 95% attendance rate - Very positive feedback



My Method of Overall Assessment

- Students have a **two-hour lab test** toward the end of the course
 - Need **students to prove individually** they can use Aspen Plus to solve problems
 - **They know its coming from day one** so they know they have to keep up
 - All 120 students **take at the same time**
- **Use 5-Tier Strategy**
 - Students get points for highest tier completed

Tier 1
10/50 points

- Push the buttons on a straightforward example

Tier 2
20/50 points

- String a few models together
- Solve a basic problem that doesn't require advanced tools

Tier 3
30/50 points

- Solve a meaningful problem that requires basic tools

Tier 4
40/50 points

- Expand on Tier 3 for a more complex problem
- Requires advanced tools

Tier 5
50/50 points

- Expand on Tier 4
- Requires a complex combination of advanced tools

Tiered Test Strategy

Disadvantages	Advantages
Have to teach students about the tiered structure, and how to use it to their advantage	Weaker students can focus on demonstrating at the level they know , rather than hoping for partial credit
Can be tricky to make a tiered test	Stronger students can jump directly to the middle of the test
	Grading significantly easier : grade highest tier submission and only more if needed
	Good when time constrained: time spent on critical thinking rather than racing through a simulation
	Lower student anxiety
	Student feedback is consistently positive with this method

Tiered Test Example

Tier 1

FIND THE OUTPUTS OF USING A PUMP

Determine the amount of electricity it takes to pump 100 kmol/hr of an equimolar mixture of n-hexane and n-heptane from 25°C and 1 bar to 1.5 bar, using default efficiency settings. Also, report the temperature of the liquid after pumping

Tier 2

MODEL A COMBUSTION REACTION

Suppose 25 kmol/hr of methane and 1000 kmol/hr of air (both at 25°C and 1 bar) are combusted in an adiabatic combustion chamber to 100% completion. Then suppose the hot exhaust gases are used to heat up a 100 kmol/hr of an equimolar mixture of n-hexane and n-heptane (also at 25°C and 1 bar), which completely vapourizes it and superheats it. The cooled exhaust gases leave at 250°C. Find the temperature of the hexane/heptane mixture after it is heated.

Tier 3

DESIGN A DISTILLATION COLUMN

Design a distillation column that separates a mixture of 50 mol% n-hexane, 50 mol% n-heptane (total flow of 100 kmol/hr at 1.5 bar and 25°C) into 98 mol% pure n-hexane and 98 mol% pure n-heptane. The target distillate and bottoms purities should be achieved within 0.01 mol%,

Tier 4

TIER 3 + HEATING/COOLING/PUMPS. UTILITY COSTS.

Complete Tier 3, and add heat and pressure management system to get distillation and bottoms products to storage conditions (35°C, 1.5 bar). Compute total utility costs in each category in \$/hr.

Tier 5

TIER 4 + ADD ECONOMIZER AND OPTIMIZE SYSTEM .

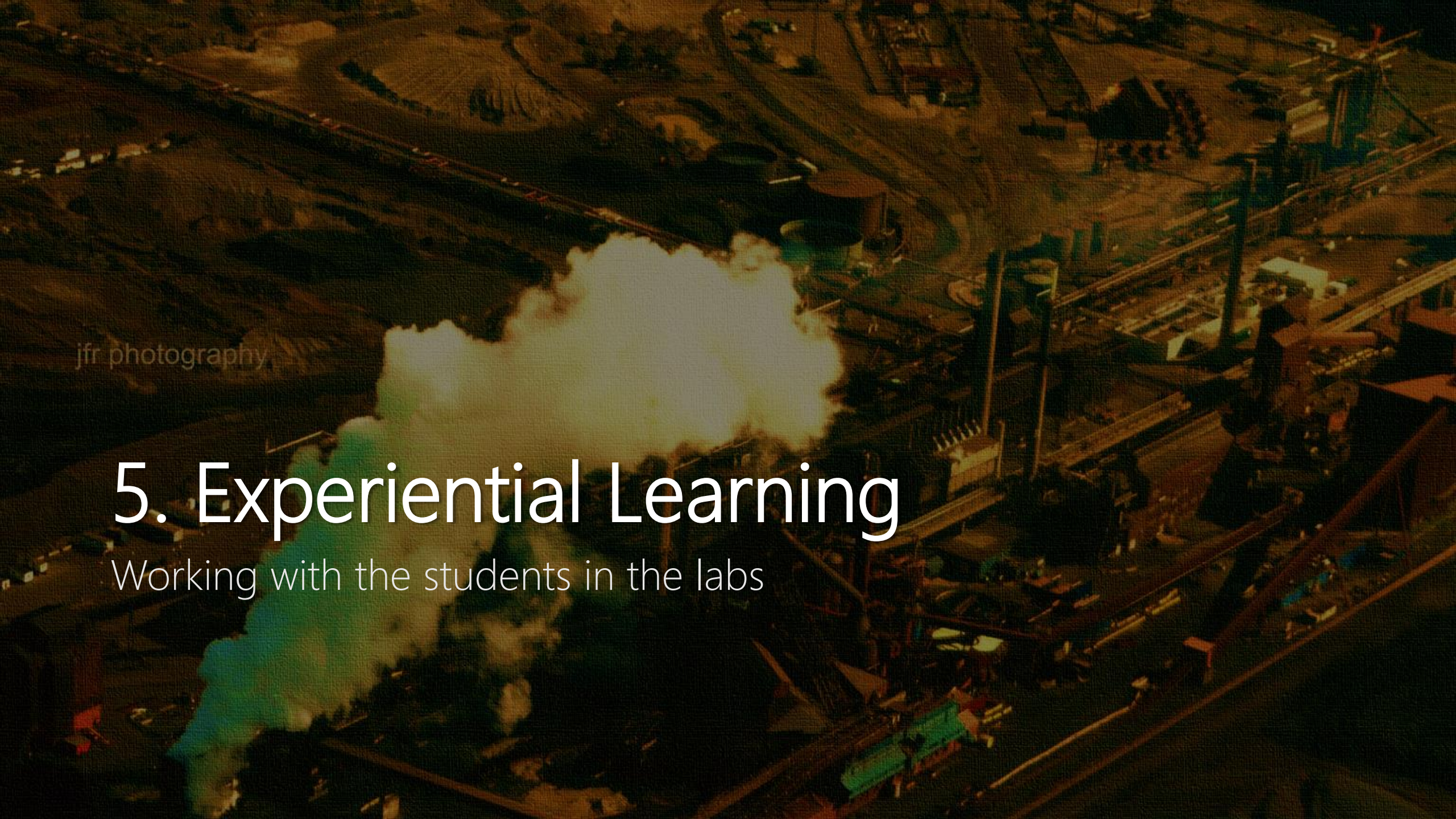
Complete Tier 4, Then, improve upon the process design by using an economizer. Use Aspen Plus to find the optimum heat duty of that economizer, which is the heat duty which makes the total utility costs the lowest. The approach temperature in the economizer should not be smaller than 5°C,

Integrating Piecemeal / Curriculum Integration

- Allow time for students to watch pre-requisite videos, etc. for preparation.
- May need to modify / skip sections that use advance features if done out of order.
- **Recommended:** have students use Access Engineering to download individual chapters instead of purchasing hardcopy

Example Use by Course

Course	Recommended Chapters
Mass Balances	Introduction, 1
Energy Balances / Heat Transfer	Introduction, 1, 4.1, 4.2, 11
Thermodynamics	Introduction, 1, 2, 12.3
Separations / Distillation	Introduction, 1, 2, 7, 8
Reactions / Reactors	Introduction, 1, 6
Engineering Economics	Introduction, 1, 10
Solid Processes	Introduction, 1, 12.1, 12.2
Optimization	Introduction, 1, 11
Process Modelling & Simulations	Entire book
Process Design / Capstone	Entire book

An aerial photograph of an industrial facility, possibly a refinery or chemical plant. The scene is dominated by a large, billowing plume of white smoke or steam that rises from the center-left area. The ground is a complex network of pipes, walkways, and industrial structures. In the background, there are large storage tanks and more industrial buildings. The overall color palette is dark and industrial, with the white smoke providing a stark contrast.

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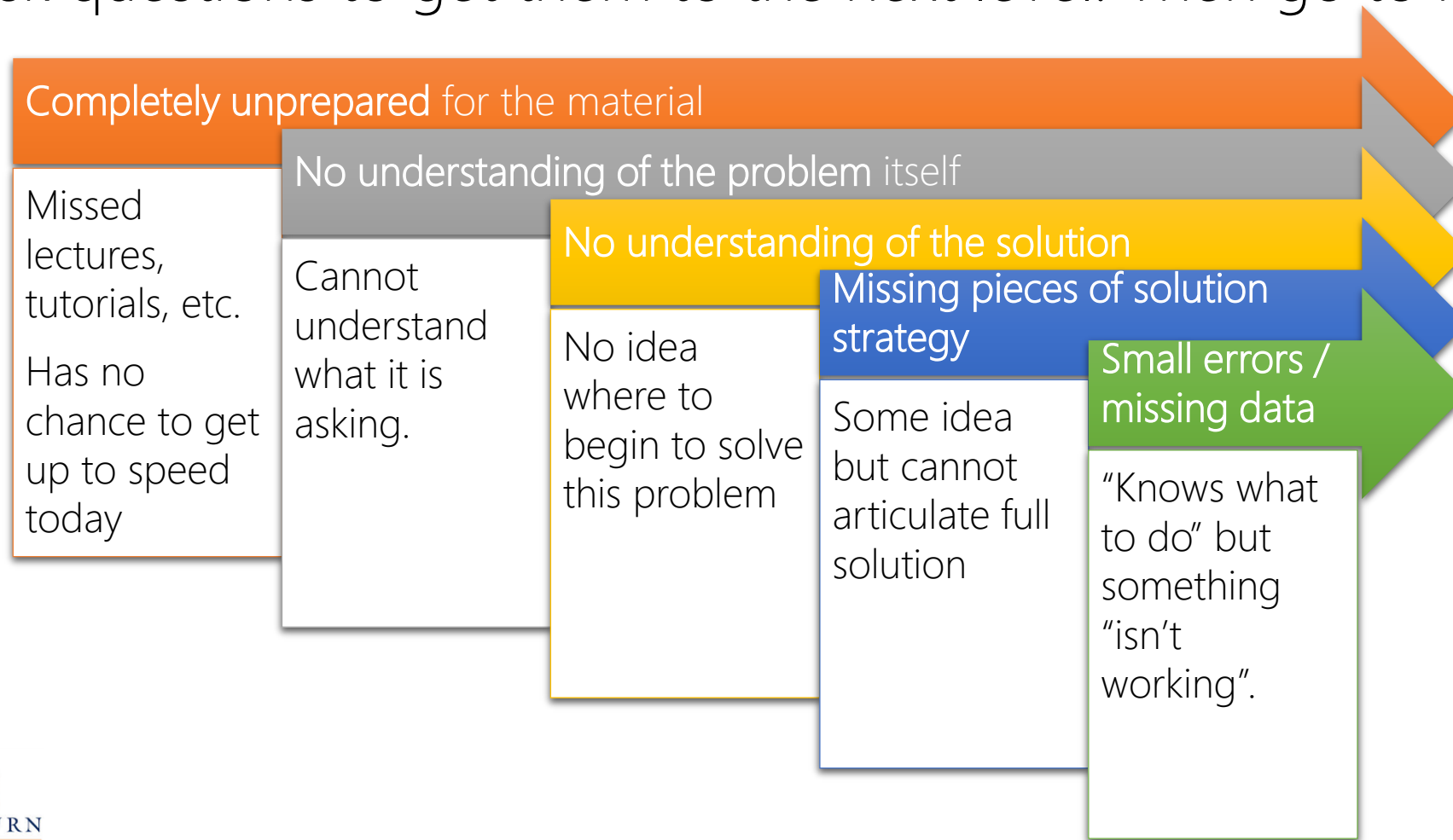
5. Experiential Learning

Working with the students in the labs

Engaging Students for Problem Solving

STEP 1: Ask questions to assess their knowledge level.

STEP 2: Ask questions to get them to the next level. Then go to next student.



What to do at Level 1 (Completely unprepared)

Completely unprepared for the material

- Currently in the lab / tutorial:
 - Politely advise the student to do some specific preparation (reading, etc.) so they can get ready to tackle the tutorial.
 - Direct them to the "Prerequisite Knowledge" section and have them watch the linked videos
 - You will be happy to help when they are ready

What to do at Level 2 (Don't understand problem)

Completely unprepared for the material

No understanding of the problem itself

- Try to re-explain problem in a different way
- Talk about what kinds of solutions it requires (Ex: "The problem is asking which heat exchanger design is more profitable. What kind of numbers do you need in order to show that?")
- Ask them to consider a simple version of the problem and then build upon that (Ex: "How would I know if a single heat exchanger requires a lot of energy?")
- Ask: "Are there phrases or terms that you specifically do not understand?"

What to do at Level 3 (Don't understand solution)

Completely unprepared for the material

No understanding of the problem itself

No understanding of the solution

- Start the conversation: "What ideas have you thought about so far?"
- Ask: "What do think a correct answer might look like?" (Ex: A temperature between 50 and 65°C)
- Ask: "What are some of the key concepts that you think you need for this problem? (example, mass balances, integrate an equation, etc.)"
 - Can you explain knowledge gaps quickly?
 - If not: point them to resources for those
- Get them to articulate the solution strategy

What to do at Level 4 (Small Strategy Gaps)

Completely unprepared for the material

No understanding of the problem itself

No understanding of the solution

Missing pieces of solution
strategy

Small errors /

Ok to clue them in more at this stage.

- Ask: "What have you tried so far?"
- Focus on the specific knowledge gaps
 - Do they just need a quick reminder?
 - Ask them to come up with some strategy options and give their thoughts on each (offer some yourself that include the right one)
- Ask them to draw out all the steps involved

What to do at Level 5 (Small Data Gaps)

Completely unprepared for the material

No understanding of the problem itself

No understanding of the solution

Missing pieces of solution
strategy

Small errors /
missing data

Can be simple and direct at this stage.

- "Oh, that's in the Pressures tab of the form"
- "Oh, you just need the `fprintf` function for that."
- Ask: "Any idea of which step you went wrong?"
- Suggest tests they can do to identify the error. "Do a mass bal. around each box until something's off."

Remember

- Students learn so much more when they connect the dots themselves
- If you are just a data source for answers, they will never stop asking you...
- If you have TAs, train them to do the same thing as you would do.
 - I found that with TAs who had at least 1 year of using Aspen before, I didn't have to be in tutorials at all after week 2 or 3.

Tips: Engaging Students in Tutorials and Labs

- No one asking questions for long periods? Don't just sit there!
 - Are students collaborating in a group? **Actively listen.**
 - Are they totally on the wrong track? **Ask some starter questions** to get them righted.
 - Did a student come up with a good idea? **Encourage them to explore that idea?**
 - Are students arguing over competing ideas? **Moderate an intelligent discussion.**
 - **"So, how are you trying to solve this problem?"**
 - **"What success have you had so far in solving this problem?"**
 - **"What are your ideas so far?"**
 - But don't be annoying
- **Beware Time Burglars** → Students who try to monopolize all your/TA's time
 - Spend 1-2 minutes per student at a time. Then break and leave.
 - If no hands go up then you can go back to that student again.



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6. Graduate Education

Graduate Student Training

- New grad student that needs to learn Aspen Plus? Give them the book.
 - A grad student should be able to teach themselves from the book without requiring your interference
 - We've done this many times in many different groups.
- Integrating into graduate courses?
 - Tell us how you did it!
 - Tom uses it as prerequisite material for grad courses in Aspen Dynamics and Aspen Custom Modeller.



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7. Workshop 2

Workshop 2

- Continue with your tutorial or switch
- Think about how your students will be using the book and what kinds of questions they'll be asking.

An aerial photograph of an industrial facility, possibly a refinery or chemical plant. The image shows a complex network of pipes, storage tanks, and industrial buildings. A large, dense plume of white smoke or steam rises from the center of the facility, partially obscuring some of the structures. The overall color palette is dominated by dark, muted tones, with the white smoke providing a stark contrast.

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8. How to Get Help

What to do if you are not an expert

- Start by **doing the book** yourself
- Then spend some time with the **user guide** for specific unit operation models of interest.
 - Don't spend much time on the physical properties details
 - Don't focus on advanced tools, just the basic unit operation models.
- The software comes with **many example files**
 - Good for **seeing working examples**
 - **Bad for learning how to get things to converge** (they come already-solved)
- **Keep your expectations low** for your students
 - K.I.S.S.!
- Stick to application examples **in your wheelhouse** (biofuels, polymers, etc)

Installation, Setup, Licenses, Etc

- support.aspentech.com
- Have an IT person handle all the logistics for you!
- Admittedly can be difficult to install software and license server

Software Usage Issues / Best Practices

- AspenTech's official community:
<http://www.aspentech.com/Community/Discussion/>
- LinkedIn AspenTech Group very helpful
- New CAChE CAPE community discussion boards.
 - <http://PSECommunity.org>
 - Will have some videos as well!



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9. Accessing Resources

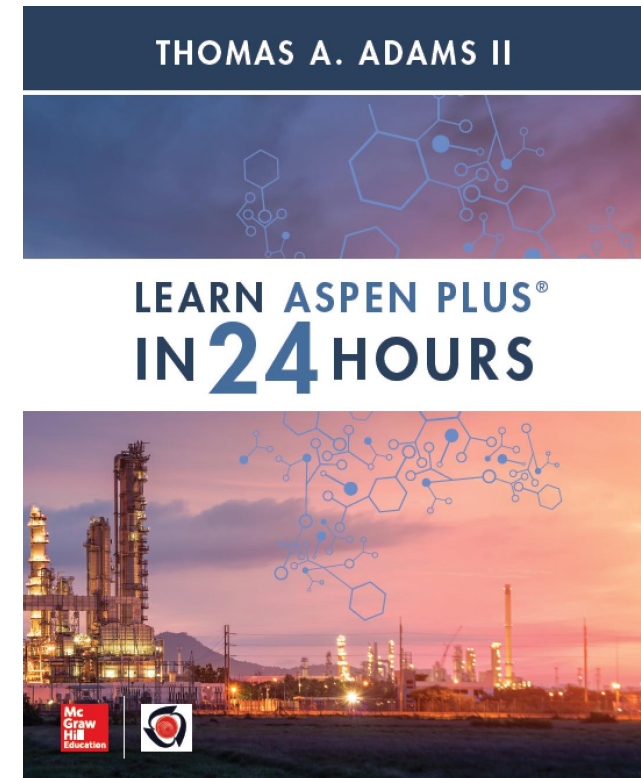
How to Order for Your Courses

- **Instructors**

- To order **examination copy**: MHPProfessional.com/examcopies
- **Download simulation files** (solutions): PSECommunity.org/books/lap24
- See flyer included in digital handouts for **discount promo codes**

- **Students and Professionals**

- **Print Edition \$60** from McGraw-Hill: ISBN: 978-1-260-11645-8
 - Give this number to your campus bookstore
 - Students can also order from Amazon and Barnes & Noble
- **E-book \$??** (PDF, Virtual Bookshelf, etc.) from McGraw-Hill
- **HTML Version** on Access Engineering: **Free to subscribers!**
 - All **CSCHE** Members
 - Many universities via library login / Campus IP address
- Available Sept 2017



Simulation Files and Samples

- All simulation files available at:
 - <http://macc.mcmaster.ca/LAP24.php>
- Additional simulation files on CO₂ capture at:
 - <http://macc.mcmaster.ca/solventsims.php>

How can you contribute?

- Write your own modules, tutorials, and chapters
 - Can publish and peer review on new online community
 - PSEcommunity.org
- Write similar texts for other software

GOOD LUCK!