ASPEN Tutorial

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Outline

• (Re)Learn the Basics & Prep for Examples
  • Components and Flowsheet Setup
  • Property Package Selection

• Two Example Problems
  • Flash Drum Performance
  • Distillation Column - shortcut and rigorous methods

• Sensitivity Analysis

• Estimating Transport Properties and Thermo

• Challenge Problems
The Basics

- ASPEN is a simulation engine that doubles as a giant thermo database.
- We use it for complicated thermo problems and process design.
The Basics

• Component Setup
  • What substances do you have?
• Property Package Selection
  • How do you want to model them?
• Flowsheet Setup
  • What units are you simulating?
Component Setup

• This is where you add the substances you’re dealing with.

• Global - you do this once, not for each block.

• Just search through the list and add everything you want.
Property Package Selection

- This is where all the thermo is specified.

- There are options like Ideal Raoult’s Law, van Laar, NRTL, Peng-Robinson, etc.

- Check your problem statement for:
  - Ideal System?
  - Equation of State given?
  - Activity Coefficient Model specified?
  - Do you have a special system with special thermo?

- If you don’t have any of those, then go through the flowcharts on Dr. Ring’s presentation - click EXERCISE_02 Choosing..> or find it on http://www.che.utah.edu/~ring/Process%20Simulators%20in%20Che3853%20Thermo/
Flowsheet Setup

- Here you add the units and material streams you want.

- The symbol is not the unit! Check the name before adding.

- If you need to reroute a material stream, use the Reconnect button on the toolbar.
Flowsheet Setup

• Until you are more familiar with ASPEN and the unit you’re simulating, use the magical green arrow to do unit specs and stream definitions.
Example I: Flash Drum

- As you know from Thermo II, flash drums in ASPEN are pretty straightforward.
- This example will be quick, but we’ll come back to it later with sensitivity analyses and transport property estimation.
- Follow along so you can have it ready when the time comes for new material.
Example I: Flash Drum

Problem Statement

- Separate 100 kmol/hr of a liquid mixture of ethanol (40%) and water at 101.3 kPa.

- Let \( V/F = 2/3 \), and the flash drum operates at 101.3 kPa.

- Find the ethanol mole fraction in the vapor and liquid products
Example 1: Flash Drum Property Package

- Going through the flowchart (Carlson)
  - Polar
  - Non-electrolyte
  - $P < 10$ bar
  - Interaction Parameters available
  - Liquid-Liquid? Either way we can use NRTL or UNIQUAC
Screenshot of property package selected.

Circle NRTL
Example I: Flash Drum

Flowsheet Setup

• Add a Flash2 block, with one inlet and the two outlets.

• For the Feed stream input:
  • 101.3 kPa pressure
  • 0 vapor fraction (specified as pure liquid input)
  • 100 kmol/hr, 60% water, 40% ethanol

• For the Flash Drum input:
  • 101.3 kPa pressure
  • V/F = 2/3 = 0.6667 is the vapor fraction
In the Aspen Plus V7.3.2 - aspenONE software, the flash specifications for the DRUM (Flash2) are set. The flash type is specified as Pressure and Vapor Fraction. The pressure is set to 101.3 kPa, and the vapor fraction is 0.6667. The valid phase is set to Vapor-Liquid.
Example I: Flash Drum Simulate

• Now just press run!
• Click “Custom Stream Results” in the Drum Block (left-hand-side).
• EtOH Fractions: 16.6% in L, 51.7% in V
• Save the simulation, we’ll come back to it later. Save as a .apw file!
Select and copy the stream table - it will paste directly into Excel!

With custom stream results you can change units! This matters when you want awkward units like SCFs.
Example II: Problem Statement

- **Distillation of acetone and ethanol**
  - 100 kmol/hr of acetone (60%) and ethanol (40%)
  - Feed is a saturated vapor at 1 atm
  - We want distillate fraction 98% acetone, bottoms fraction of 1% acetone
  - Column has reflux ratio $R = 2$, total condenser, kettle reboiler

- **Tasks/Questions:**
  - Plot the x-y diagram with ASPEN
  - How many stages should we have?
  - Where should the feed enter the column?
  - What is the minimum number of stages?
Example II: Pre-ASPEN Work

- Always do the overall and component mass balances first! Find D and B in this problem.
  - D = 60.8 kmol/hr
  - B = 39.2 kmol/hr
- Use these to compute recoveries. ASPEN defines recovery as the amount of component in the distillate divided by the amount of component in the feed.
  - Light key (acetone) recovery = 99.3%
  - Heavy key (ethanol) recovery = 3.04%
- Gotta know the thermo: NRTL will work for acetone/ethanol
- How are we going to do this in ASPEN?
  - Start with ASPEN's shortcut distillation column
  - Finalize with ASPEN's rigorous distillation column
Example IIa: Shortcut Distillation Column

- DSTWU is ASPEN’s block for shortcut methods (Gilliland, Underwood, Winn)
- It is generally used as a starting point, since more complicated methods require more complicated input
- Use DSTWU to start a design problem
- Don’t use DSTWU for a spec problem
Feed Stream Input

- Pressure and Vapor Fraction specified
  - 1 atm and saturated vapor

- Flow rate specified
  - 100 kmol/hr

- Composition Specified
  - Acetone mole frac = 0.6, Ethanol mole frac = 0.4
DSTWU Input

• Either number of stages or reflux ratio
  • \( R = 2 \) specified

• Condenser and reboiler pressures
  • 1 atm (based on feed pressure)
  • Assume no pressure drop over the column

• Condenser type
  • Total condenser specified

• Light and heavy key recoveries
  • 0.9931 light key, 0.0304 heavy key
DSTWU Results

- Minimum and Actual Reflux Ratio
- Minimum and Actual Number of Stages
- Feed Stage (for actual number specified)
- Reboiler/Condenser heat duties
- Distillate, Bottoms Temperatures
- Distillate to Feed Fraction

- Don’t forget Custom Stream Results
**DSTWU results section**

Circle the values

Note the exact agreement with our hand-calc. DSTWU enforces this. It doesn’t mean anything!
DSTWU Answer

• Minimum number of stages: 15
• Real number of stages: 145
• Feed Stream: 89

• Not done yet...
Getting the x-y Diagram

• To get the x-y diagram, go back to the Properties window, and find the “Binary” button with a graph icon next to it. (upper right)

• Select a Txy analysis type.

• Default parameters should be fine in most cases.
Example IIb: Rigorous Distillation Column

- RadFrac is ASPEN’s block for rigorous methods
- It is difficult to start with RadFrac without having first done a shortcut method like DSWTU.
- RadFrac is great for spec problems, but requires iteration for design problems.
- Accuracy is worth it.
RadFrac Input

- **Calculation Type:** Equilibrium
- **Number of Stages:** 145 stages from DSTWU
- **Condenser Type:** total condenser specified
- **Reboiler Type:** kettle reboiler specified
- **Valid Phases:** vapor-liquid
- **Convergence:** standard
- **Operating Specs x 2:**
  - distillate rate = 60.8 kmol/hr from initial calcs and DSTWU
  - reflux ratio = 2 specified
- **Feed Stream Location:** Stage 89 from DSTWU
- **Condenser Pressure:** 1 atm specified/inferred
RadFrac Results

- RadFrac outputs... a lot.
- First of all, check the Stream Results
  - Note that they are not the same!
- Next check out the RadFrac block results.
  - Look to the top-right part of the screen and you’ll see the ability to plot things
  - Try making a plot of acetone composition in the vapor over stage number
<table>
<thead>
<tr>
<th>Component Mole Flow</th>
<th>Units</th>
<th>B</th>
<th>D</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACETONE</td>
<td>KMOL/HR</td>
<td>1.846e-15</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>ETHANOL</td>
<td>KMOL/HR</td>
<td>39.2</td>
<td>0.8</td>
<td>40</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>KMOL/HR</td>
<td>39.2</td>
<td>60.8</td>
<td>100</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>KG/HR</td>
<td>1805.91</td>
<td>3521.66</td>
<td>5327.56</td>
</tr>
<tr>
<td>Volume Flow</td>
<td>L/MIN</td>
<td>41.0371</td>
<td>78.1923</td>
<td>46229.4</td>
</tr>
<tr>
<td>Temperature</td>
<td>°C</td>
<td>78.3103</td>
<td>56.2452</td>
<td>64.883</td>
</tr>
<tr>
<td>Pressure</td>
<td>BAR</td>
<td>1.01325</td>
<td>1.01325</td>
<td>1.01325</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td></td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Liquid Fraction</td>
<td></td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Solid Fraction</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Molar Enthalpy</td>
<td>CAL/MOL</td>
<td>-64531.2</td>
<td>-58084.1</td>
<td>-52652.3</td>
</tr>
<tr>
<td>Mass Enthalpy</td>
<td>CAL/GM</td>
<td>-1400.75</td>
<td>-1002.8</td>
<td>-988.3</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>CAL/KG</td>
<td>2920.86</td>
<td>0</td>
<td>1428.05</td>
</tr>
</tbody>
</table>
Note the axes! A column is oriented vertically, so put the stages on the y-axis in descending order.
RadFrac Answer...

almost

• This is going to be tricky... we’re going to have to try a bunch of values until we hit the right results.

• Remember we’re trying to find min. number of stages, actual number of stages, and optimum feed stage.

• Let’s try playing with the number of stages and checking against the acetone flow rate in the distillate. At 98%, it should be 59.6 kmol/hr

• Look at the comp. profile to get an idea for your next estimate.
RadFrac Answer...
almost

<table>
<thead>
<tr>
<th>Nstages, Feed Stage</th>
<th>Acetone flow in distillate (kmol/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>145, 89</td>
<td>60</td>
</tr>
<tr>
<td>50, 39</td>
<td>59.9</td>
</tr>
<tr>
<td>30, 20</td>
<td>58.9</td>
</tr>
<tr>
<td>30, 10</td>
<td>56.5</td>
</tr>
<tr>
<td>30, 25</td>
<td>59.2</td>
</tr>
<tr>
<td>40, 30</td>
<td>59.6</td>
</tr>
</tbody>
</table>
RadFrac Answer...
almost

- To find min. number of stages, remember that we get that number by setting reflux ratio to infinity.
- Set \( R = 1000 \) or some large number
- Then play with \( N \) stages, start around the 14 we got from DSTWU
RadFrac Answer...
almost

<table>
<thead>
<tr>
<th>Nstages, Feed Stage with R = 1000</th>
<th>Acetone flow in distillate (kmol/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14, 8</td>
<td>59.8</td>
</tr>
<tr>
<td>8, 5</td>
<td>57.3</td>
</tr>
<tr>
<td>10, 5</td>
<td>58.7</td>
</tr>
<tr>
<td>14, 5</td>
<td>59.8</td>
</tr>
<tr>
<td>12, 5</td>
<td>59.5</td>
</tr>
<tr>
<td>12, 1</td>
<td>59.4</td>
</tr>
<tr>
<td>12, 11</td>
<td>59.5</td>
</tr>
<tr>
<td>12, 9</td>
<td>59.5</td>
</tr>
<tr>
<td>13, 5</td>
<td>59.7</td>
</tr>
</tbody>
</table>
RadFrac Answer... finally

- Minimum number of stages: 13
- Real number of stages: 40
- Feed Stream: 30

Yes, there is a better way to do these problems with RadFrac!
Sensitivity Analysis

- This allows you to automatically perform the simulation over a range of a parameter, and output specified variables for each result.

- This is VERY useful in design problems, since you can get a plot of design metric(s) over design parameter.
Sensitivity Analysis

- **Without** this, you’re left attempting an initial guess and trying new values until you get the correct results.

- **With** this, you can interpret and solve the problem graphically, as opposed to random sampling and mental bisection.
Sensitivity Analysis

• Be cognizant of your parameter ranges. Remember the bounds of applicability on your property package (i.e. P < 10 bar?)

• Even if your property package should work, always be careful with extreme parameter values.
Sensitivity Analysis for Extension of Problem 1

• Previously, Problem 1 (the flash drum) was easy and only required one iteration. Senior Design problems either don’t start this way or won’t stay there for very long!

• Now you’ve been asked to find the value of $V/F$ required to obtain an ethanol mole fraction of 60% in the vapor product.

• You could guess and check, or you could just do a sensitivity analysis.

• Sensitivity Analysis is faster and provides more information.
After this, go to the “Tabulate” section and just press “Fill Variables”.
After this we went to the Results of the Sensitivity Analysis and found “Results Curve” on the top-right.

Now you know a ballpark value. Test more in that area to get a more detailed answer.

V/F = 0.23
Sensitivity Analysis for Solution of Problem II

• Remember the awful iterations we did for problem II with RadFrac?

• We still have to be smart, but sensitivity analyses can really reduce our work load (and related mental effort).

• This problem is a little tricky since we have both the feed stage and the number of stages to vary, but sensitivity analysis can help immensely.
Sensitivity Analysis for Solution of Problem II

• Let’s go back to the problem with R = 2. How many stages and where is the best feed stage?

• We have a bivariate problem - unfortunately we still have to play with one variable.

• Because feed stage possibilities are restricted by number of stages, we will play with the number of stages, and do sensitivity analysis over feed stage.

• In bivariate problems like this, identify before doing anything what variable to play with and what variable to use sensitivity analysis on.
Looking at the composition profile we printed out for 145 stages, you can see that about 100 stages don’t really do much.

Let’s start with 40 total stages and vary the feed stage from 1 to 39.
You can make the plots look better with the format toolbar.

Acetone mole fraction in distillate stream, plotted over feed stage for 40 total stages.
Sensitivity Analysis for Solution of Problem 11

- 40 stages worked, but just barely.
- Let’s see if we can go down to 35 total stages.
You can make the plots look better with the format toolbar

Acetone mole fraction in distillate stream, plotted over feed stage for 35 total stages
Sensitivity Analysis for Solution of Problem II

- Clearly we need more than 35 stages.
- You could try 36-39 but 40 is accurate enough.
- Now we’ve already arrived at an answer (40 stages, feed on stage 30) and it didn’t require much luck in our guesswork.
- And we’ve also got plots of what happens to distillate quality as we vary feed stage.
Estimating Thermo and Transport Properties

- ASPEN allows you to estimate properties like density, viscosity, specific heat capacity, and thermal conductivity.

- You can also get dew/bubble point curves, PV curves, etc.

- This isn’t automatic but is very useful. Particularly when you design things (i.e. shell-and-tube heat exchangers) that need a lot of transport properties.
Estimating Thermo and Transport Properties

• Go back to our friendly Flash Drum from Problem I.
• Find the Stream Analysis -> Point button
The image shows a computer screen with a software interface open to the 'Stream Analysis' section. The interface is part of a simulation software, likely used for chemical engineering simulations. The screen displays various data points related to a stream analysis, including temperature, pressure, composition, and other properties. The data is presented in a table format with columns for different properties and rows for specific data points.

### Table Example

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>F</td>
</tr>
<tr>
<td>Pressure</td>
<td>BAR</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>0</td>
</tr>
<tr>
<td>Liquid Fraction</td>
<td>1</td>
</tr>
<tr>
<td>Solid Fraction</td>
<td>0</td>
</tr>
<tr>
<td>Molar Enthalpy</td>
<td>BTU/LBMOL</td>
</tr>
<tr>
<td>Mass Enthalpy</td>
<td>BTU/LB</td>
</tr>
<tr>
<td>Enthalpy Flow</td>
<td>BTU/HR</td>
</tr>
<tr>
<td>Molar Entropy</td>
<td>BTU/LBMOL-R</td>
</tr>
<tr>
<td>Mass Entropy</td>
<td>BTU/LB-R</td>
</tr>
<tr>
<td>Molar Density</td>
<td>LBMOL/CUFT</td>
</tr>
<tr>
<td>Mass Density</td>
<td>LB/CUFT</td>
</tr>
<tr>
<td>Average Molecular Weight</td>
<td></td>
</tr>
</tbody>
</table>

The interface also includes options for various analyses and simulations, such as PV Curve, TV Curve, and Point Envelope. The software seems to be designed for detailed analysis and modeling of chemical processes.
To do a different stream, go to your flowsheet, click on the stream, return to the Home section of the toolbar, and click the Stream Analysis button.