Aspen Tutorial #6: Aspen Distillation

Outline:

- Problem Description
- Aspen Distillation Options
- DSTWU Distillation
- RadFrac Distillation

Problem Description:

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams – one enriched in acetone and the other in water. The separation process consists of extraction of the acetone from the water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams which have greater than 90% purity of water and acetone respectively.

This week we will be learning about the various distillation calculation methods that Aspen uses. We will be completing the separation of our acetone/MIBK streams based on one of the simplified distillation methods, DSTWU and one of the more rigorous distillation calculation methods, RadFrac. From this we will be able to compare the results of the two distillation methods.

Aspen Distillation Options:

Aspen has multiple unit operations options for completing distillation problems, based on the complexity of the user's application. Open up your existing Aspen simulation and click on the Separators tab in the Equipment Model Library. In this tab you will see the first option that users can choose for completing a distillation process, SEP2. This unit operation can be used to model separation processes with only two possible outlet streams. This process can be used to simulate distillations, but it does not provide the level of detail that is available when using some of the other distillation options. Some key variables it does not consider include the number of trays and the reflux ratio. For this reason this option is not recommended except as a very general screening process.

Now select the Columns tab in the Equipment Model Library. You will notice a number of distillation column options. This tutorial will focus on introducing you to the three general distillation choices, DSTWU, Distl, and RadFrac. The other six unit operation choices complete much more rigorous calculations than we require for our application and they are intended for use in more difficult separations and specific applications (i.e. PetroFrac is used in simulating refining processes).

The DSTWU unit operation is designed for single feed, two product distillation processes. This column completes calculations using Gilliland's, Winn's, and Underwood's methods for calculations of stages and reflux ratios as indicated in Table 1. These calculations are completed based on two assumptions, constant molar overflow and constant relative volatilities.

Table 1: DSTWU Calculation Methods

Shortcut Method	Calculates For:
Winn	Minimum number of stages
Underwood	Minimum reflux ratio
Gilliland	Required reflux ratio for a specified number of stages or required number of stages for a specified reflux ratio

For a specified product recovery (both light and heavy), the DSTWU column first estimates the minimum number of stages and the minimum reflux ratio, and then it calculates the either the required reflux ratio or the required number of theoretical stages based on the user input. During these calculations, Aspen will also estimate the optimum feed stage location and the condenser and reboiler duties. Finally, when the calculations are complete, Aspen can produce tables and plots of the reflux ratio/stage profile. When completing complicated simulations later in your career, you could use this column to get a quick idea about a process, and use its results as inputs to a more detailed simulation.

The Distl unit operation is also designed for a single feed, two product distillation process. However, this column calculates product compositions based on the Edmister approach. Again, the calculations are completed based on the assumptions of constant molar overflow and constant relative volatilities. The user is required to input a number of the column specifications with this unit operation, including the number of stages, the reflux ratio, and the distillate to feed ratio. We will not be using this option.

The final general distillation unit operation is the RadFrac column. This distillation unit completes much more rigorous calculations than the other two methods and can be used to simulate absorption, stripping, extractive distillation, and azeotropic distillation for solids, liquids, and gases. This column can also be used for highly non-ideal liquid solutions or processes with an on-going chemical reaction. Finally, the RadFrac column can have multiple feed and product streams (including pump-around streams) and it can simulate columns with trays, random packing, or structured packing. As you can see, this distillation option is much more complicated than the previous two methods, and we will be covering this method in more depth as we input the data for it.

DSTWU Distillation:

In the last Aspen homework, we adjusted our design specification input in Tutorial #5 to achieve a water purity of 95%. We will keep this updated specification in our ongoing simulation, so if you did not complete the homework two weeks ago, do so now.

The first update we will make to our simulation is the addition of another mixer. Add in a new mixer which combines the two streams of acetone and MIBK from the two flash separators that we added in the previous tutorials. This can be seen in the process flowsheet window shown in Figure 1.
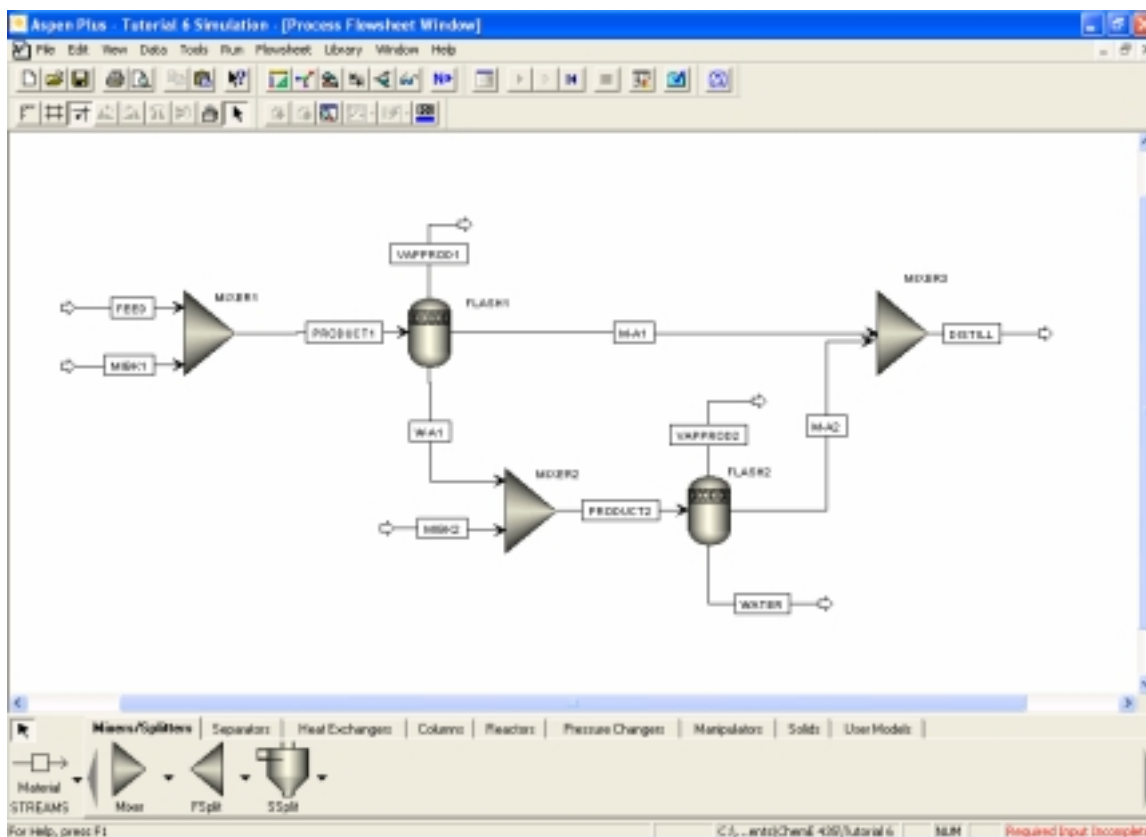
Figure 1: Acetone/MIBK Mixer

At this point save your Aspen simulation under two names. We will use one version to complete a distillation with the DSTWU distillation column and we will use the other version to complete the simulation with the RadFrac column. I would suggest saving them with names that indicate which distillation method is being used.

Now select the Columns tab in the Equipment Model Library and place a DSTWU column into the process flowsheet window. Connect the product stream from the new mixer to the DSTWU column and add in two product streams where Aspen indicates they are required. We will also be adding in a third product stream off of the condenser, to account for any free water product that can be separated from within the condenser. Rename the streams and column as you see fit. At this point your flowsheet should look similar to that in Figure 2.
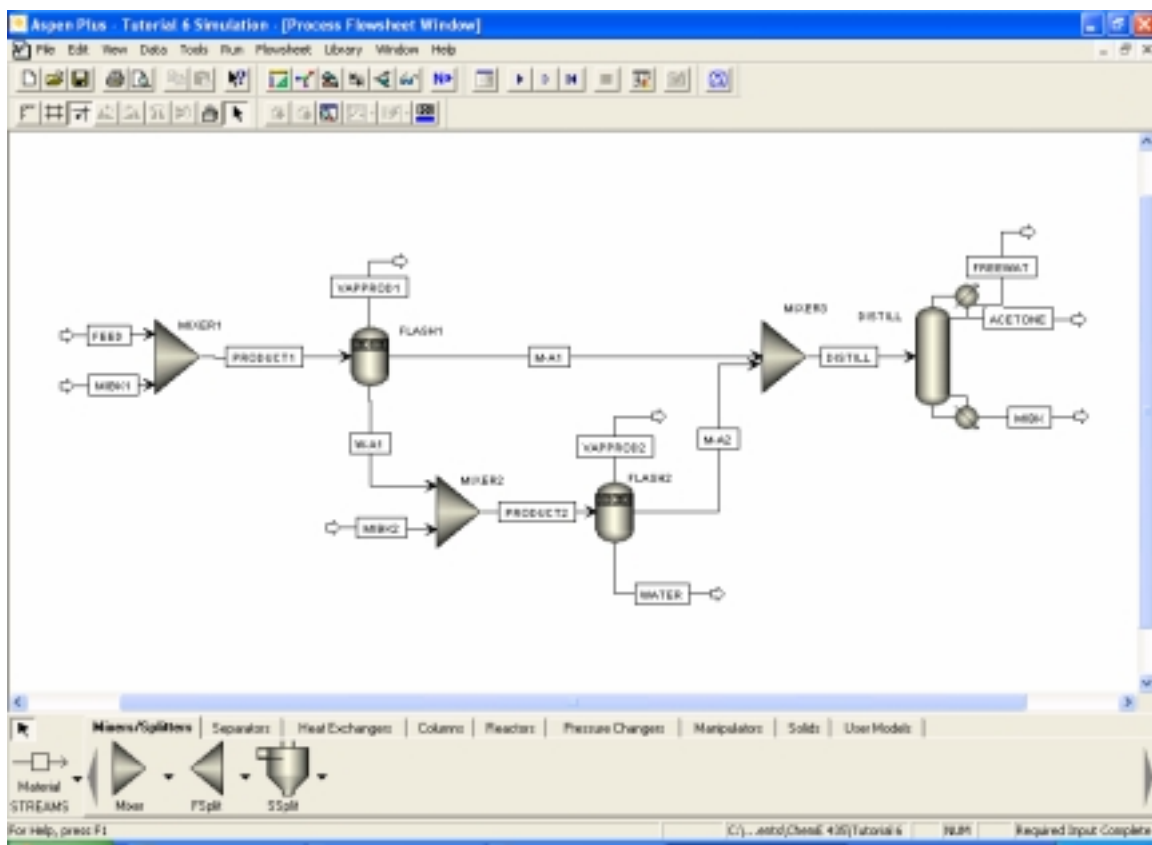
Figure 2: Completed Process Flowsheet

Now open up the Data Browser window. You will notice that we are only required to update our data input in the Blocks tab. Under the appropriate option for the new mixer, input a mixing temperature and pressure of 75º F and 50 psi. Then open up the appropriate option for the distillation column. The input window is shown below in Figure 3.
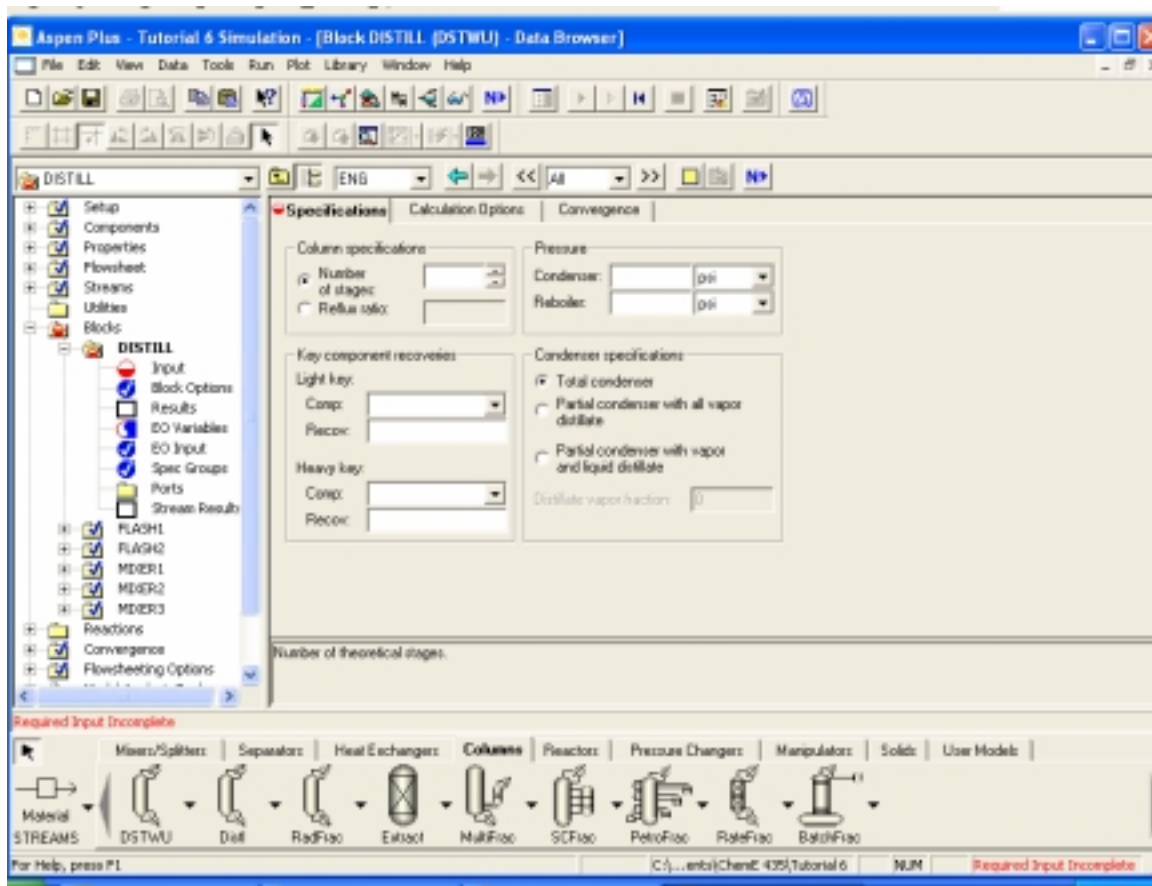
Figure 3: DSTWU Data Input Window

For this simulation we will be inputting the reflux ratio, the key component recoveries, and the tower pressures. For our purposes, we will assume that the tower has no pressure drop throughout it. However, we will set the condenser and reboiler pressures to 15 psi to aid in our separation process. We will start with an input reflux ratio of 1.5, but we will be varying this value to try and get our desired product purity. The component recovery values that are input are equal to the amount of each component in the distillate divided by the amount of each component in the feed. For this reason a recovery of 99% for acetone and 1% for the MIBK are not unreasonable if our distillation tower is operating well. The completed input screen is shown in Figure 4.
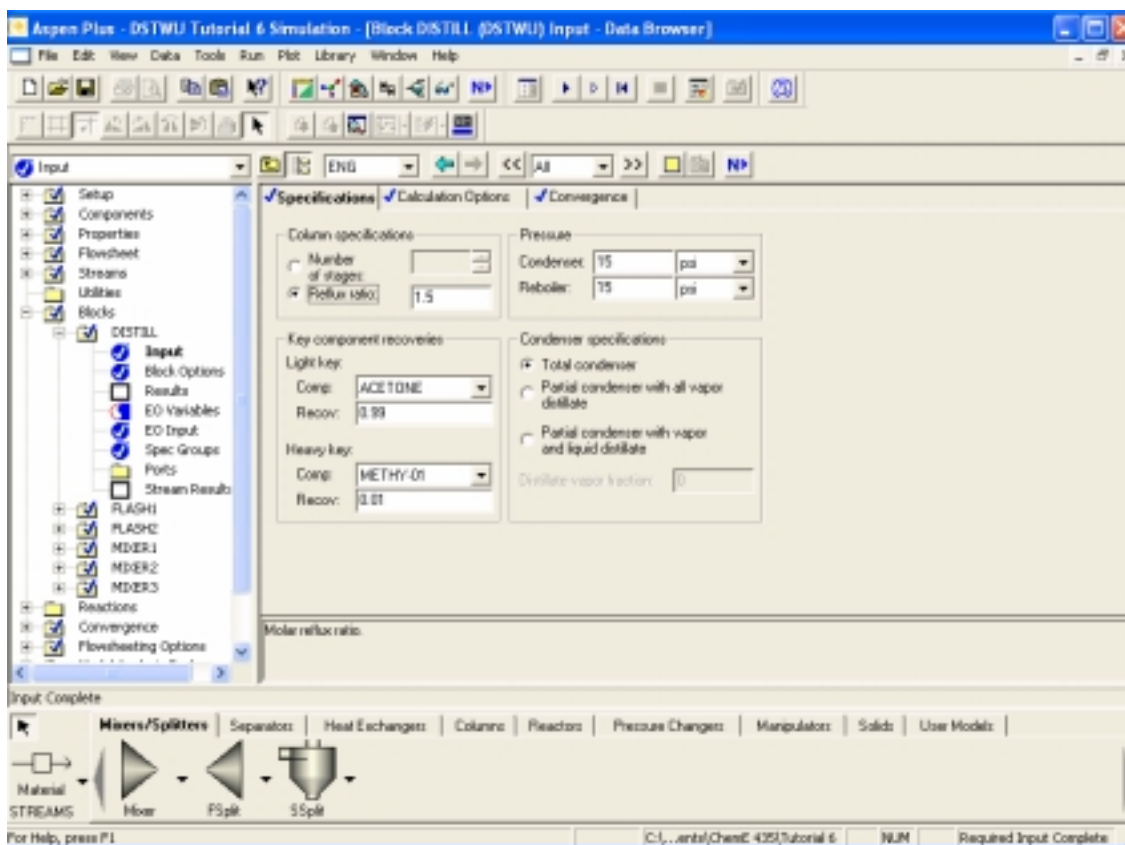
Figure 4: Completed DSTWU Input Window

For our benefit, we would also like Aspen to produce a table of reflux ratio vs. the total number of calculated theoretical trays. This can be easily done by selecting the Calculation Options tab at the top of the DSTWU input window. Check the box corresponding to this calculation now.

At this point our simulation is complete. Reinitialize and run your simulation. If you look closely at your results, you will notice that we do not achieve the desired 90% purity of acetone in this simulation. The stream table from my simulation is shown in Figure 5 where it can be seen that my simulation only achieved an acetone purity of 88%.

We can examine the reflux ratio profile for our distillation column at this time. This can be done by opening up the Data Browser window (if it is not already open) and selecting the Blocks tab. Under this tab there is an option labeled Results. Open up this window, and then select the tab at the top entitled Reflux Ratio Profile. If you were designing this tower, you could use the information in this table to determine the most cost-effective design for your distillation column. Each tray will add to the equipment cost, while the increased reflux adds to the operating costs of the column. We will use some of this information in our input for the RadFrac column.

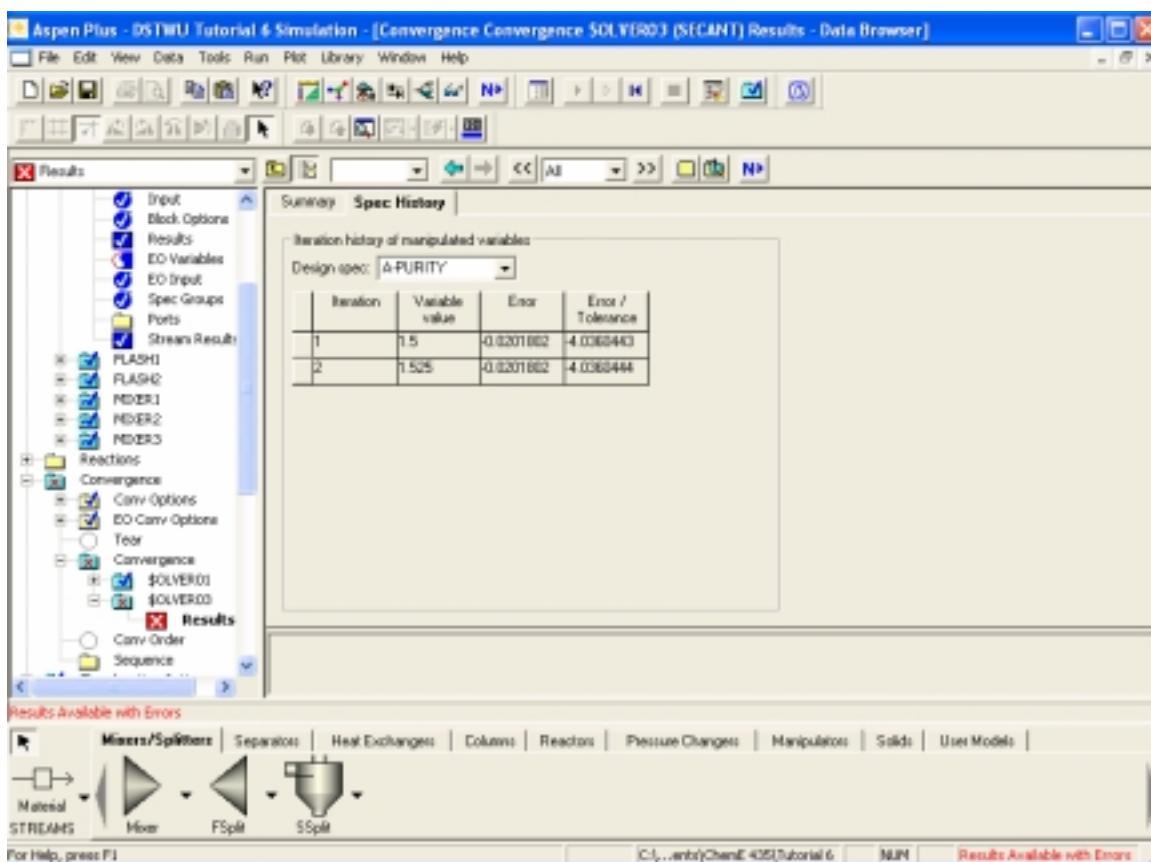| Tutorial 6 - DSTWU Distillation					
Stream ID		DISTILL	ACETONE	MIBK	FREEWAT
Temperature	F	75.2	137.0	235.2	137.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	1.006	4.253	0.514
Mass Flow	lb/hr	485.182	54.950	420.966	9.266
Volume Flow	cuft/hr	9.586	1.161	9.474	0.151
Enthalpy	MMBtu/hr	-0.771	-0.109	-0.560	-0.063
Mass Flow	lb/hr				
WATER		12.666	2.367	1.033	9.266
ACETONE		48.835	48.346	0.488	
METHY-01		423.681	4.237	419.445	
Mass Frac					
WATER		0.026	0.043	0.002	1.000
ACETONE		0.101	0.880	0.001	
METHY-01		0.873	0.077	0.996	

Figure 5: Initial DSTWU Results

Because we did not achieve the desired product purity, we will now write a design spec to try and reach our goal. Under the Flowsheeting Options tab select Design Spec and add a new one. This spec will be the calculation of the mass fraction of acetone in the acetone product stream. We will try to achieve our desired 90 wt% by varying the molar reflux ratio of the column between 0.5 and 5.0. Specify a tolerance of 0.5% for this spec. If you do not remember how to do this, refer to Tutorial #5. Hint: the reflux ratio is a Block-Var.

After you have input your design spec, rerun your simulation. In doing so, you should get an error that your Aspen simulation did not converge. Close this error message by hitting the cancel button. Because of the simplifications that are used in this type of distillation column, the purity level of our product is not affected by the reflux ratio. This can be confirmed by looking at the Convergence tab in the Data Browser window. Under this option one of the two solver files should have a red x through it. Opening up this option and selecting the Spec History tab will open up the window shown in Figure 6. You will notice in this window that the error values shown in the table do not change as the reflux ratio does, indicating that our dependent variable value is not changing.

This step was completed to provide a warning to you in your future simulation efforts. While some of the shortcut methods appear to provide a quick way to obtain results, they do not always work or provide the accuracy that is desired. For this reason we will complete the same calculations with the RadFrac column to see if the results are any different.

Figure 6: Convergence Window

RadFrac Distillation:

Close your simulation with the DSTWU distillation column and open up the second version that you should have saved earlier in this tutorial. Add in a RadFrac distillation column and three product streams as we did earlier. Your process flowsheet should again look similar to that seen in Figure 2.

Now open up the Data Browser window and the Blocks option. Input the same process design conditions for the mixer and then open up the screen related to our new column. This input window is shown in Figure 7. As you can see, this column requires a lot more input than the DSTWU column required.
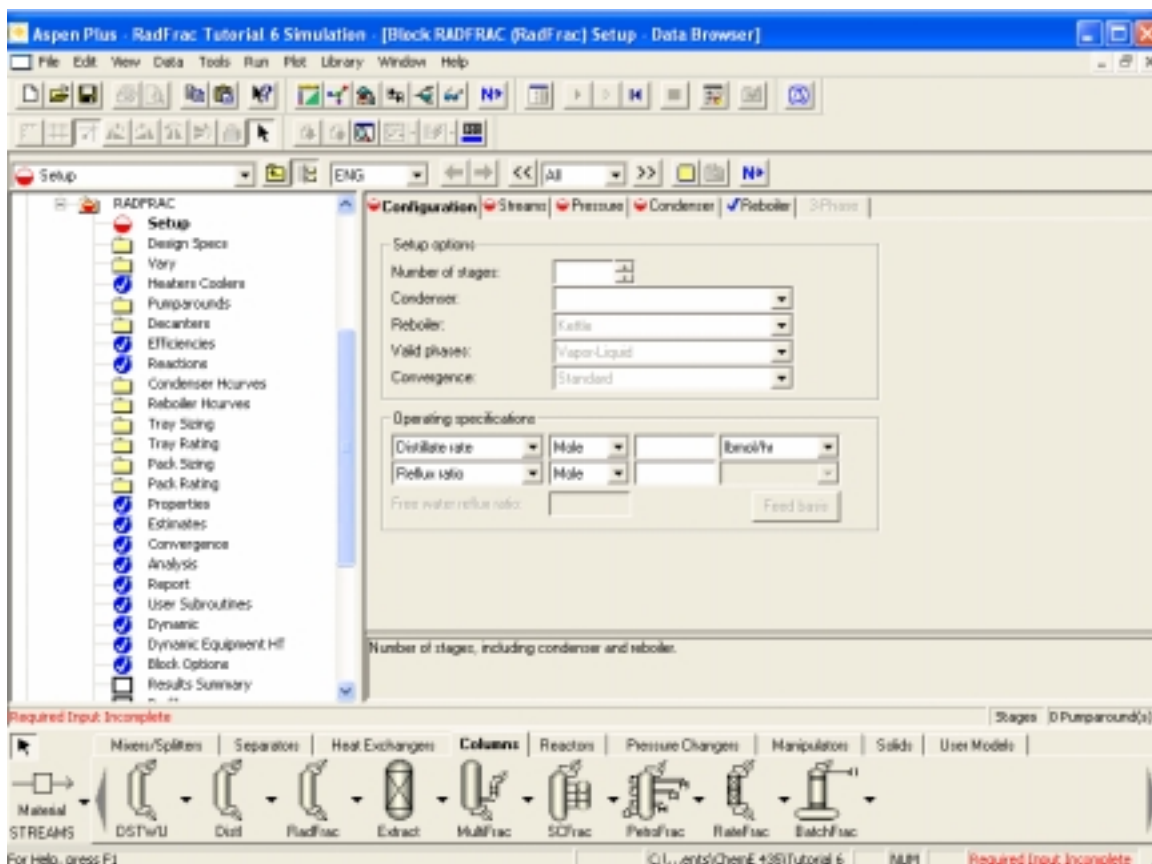
Figure 7: RadFrac Input Window

In order to compare the two distillation methods, we must input identical values into this input window wherever possible. In the Configuration tab select a total condenser, and change the valid phases to Vapor-Liquid-FreeWaterCondenser. Input a reflux ratio of 1.5 as well (molar basis). In order for us to input a specified product recovery, we must change one of the operating specifications to the option Distillate to feed ratio. However, this option is different than that for the DSTWU column and we must select the specific components that we are specifying the recovery of. To do this hit the Feed Basis button. Move acetone from the available list to the selected list under the components box and then hit the close button. Now input a recovery of 0.99. At this point we have input all of the data that was required of us for the DSTWU column (for this window), but in this case Aspen still requires more data.

You might remember looking at the reflux ratio to theoretical tray profile in the DSTWU simulation. In this profile, Aspen had calculated that 10 theoretical trays were required for a reflux ratio of 1.49. For this reason, we will input 10 trays into this simulation. At this point the input for the Configuration tab should be complete and your window should look like that seen in Figure 8.
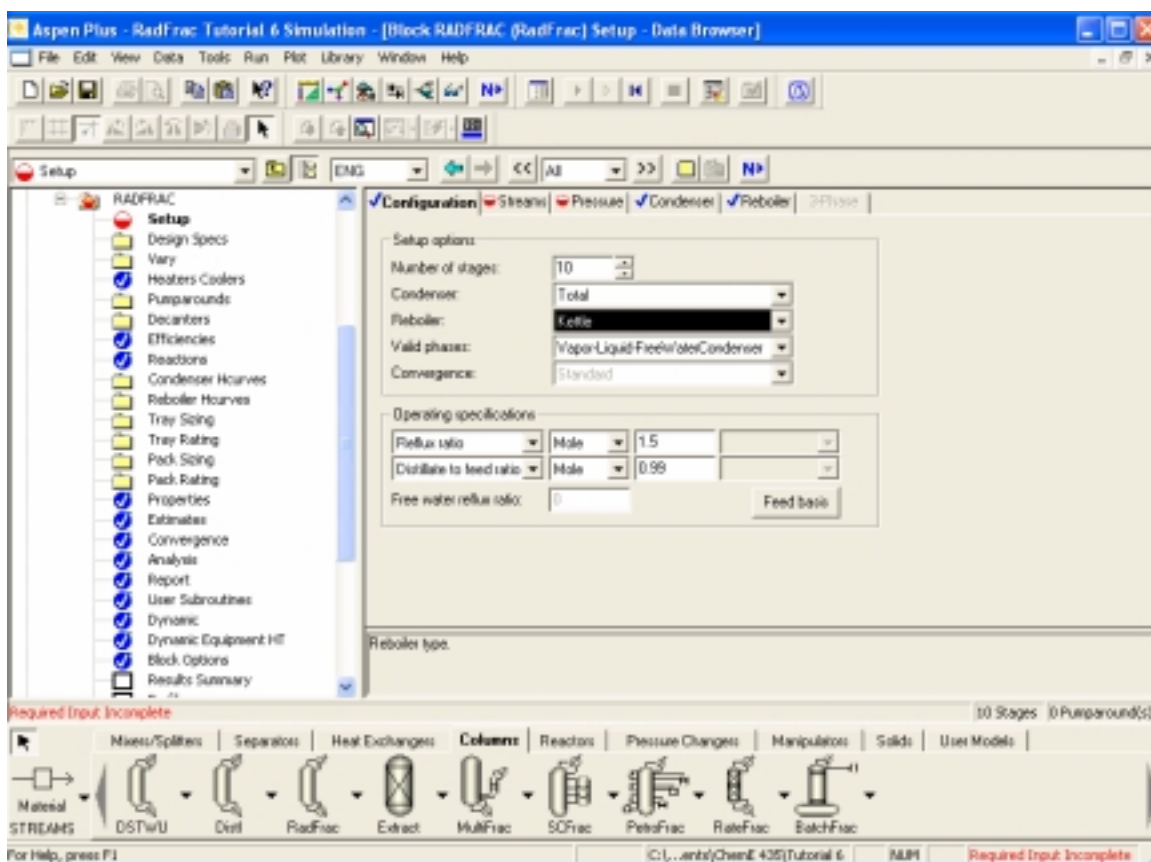
Figure 8: Completed Configuration Input

Under the Streams tab we need to input the location of the feed stream. As discussed in you mass transfer class, we will put the feed at the middle stage of the column, tray 5. In addition, your acetone stream should say 1st liquid, your water stream should say free water, and your MIBK stream should say liquid. This completes the Streams tab input. You might notice that the tray corresponding to each product stream is shown in this window. If we had any side draws from our tower or additional feeds, we would need to input which tray they occur from or to in this window.

In the final input tab, Pressure, we use the same assumption that we used in the DSTWU simulation, no pressure drop. Again, we will simulate a distillation column that is operating at 15 psi. Input this as the operating pressure at Stage 1.

At this point our required input is again complete and we are ready to run our simulation. Reinitialize and run your simulation at this point. You will notice in Figure 9 that this initial simulation actually calculates a worse purity for our acetone product than that which was obtained with the DSTWU distillation column. For this reason we will again try to input a design spec to see if we can achieve our desired 90% purity. Input the same design spec that we used in the DSTWU distillation simulation and then reinitialize and rerun your simulation.

Tutorial 6 - RadFrac Distillation					
Stream ID		DISTILL	ACETONE	FREEWAT	MIBK
Temperature	F	75.2	138.6	138.6	213.1
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	0.832	0.354	4.587
Mass Flow	lb/hr	485.182	46.466	6.379	432.336
Volume Flow	cuft/hr	9.586	0.980	0.104	9.518
Enthalpy	MMBtu/hr	-0.771	-0.091	-0.043	-0.601
Mass Flow	lb/hr				
WATER		12.666	2.021	6.379	4.266
ACETONE		48.835	38.224		10.611
METHY-01		423.681	6.222		417.460
Mass Frac					
WATER		0.026	0.043	1.000	0.010
ACETONE		0.101	0.823		0.025
METHY-01		0.873	0.134		0.966

Figure 9: Initial RadFrac Results

This time your simulation should converge, with an acetone weight percent of 90%. The results that I obtained are shown below in Figure 10.

Tutorial 6 - RadFrac Distillation					
Stream ID		DISTILL	ACETONE	FREEWAT	MIBK
Temperature	F	75.2	136.5	136.5	208.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	0.832	0.234	4.707
Mass Flow	lb/hr	485.182	45.126	4.219	435.837
Volume Flow	cuft/hr	9.586	0.954	0.069	9.532
Enthalpy	MMBtu/hr	-0.771	-0.090	-0.029	-0.618
Mass Flow	lb/hr				
WATER		12.666	1.938	4.219	6.509
ACETONE		48.835	40.596		8.239
METHY-01		423.681	2.592		421.089
Mass Frac					
WATER		0.026	0.043	1.000	0.015
ACETONE		0.101	0.900		0.019
METHY-01		0.873	0.057		0.966

Figure 10: Final RadFrac Results

As discussed in Tutorial #2, we should now check our results to make sure that they are reasonable. We will also check some of the operating parameters for the distillation column. If you look at the Run Control Panel, you will notice that the second design spec that we used took 5 iterations to converge, which is quite reasonable. Now open up the Data Browser window if it is not already open. We will look closely at the results for the

RadFrac column because this is the only significant addition to our simulation since the last time we checked the results closely. Select the appropriate unit operation under the Blocks option. Scroll down until you see the choice Results Summary and open this window. This is shown in Figure 11.
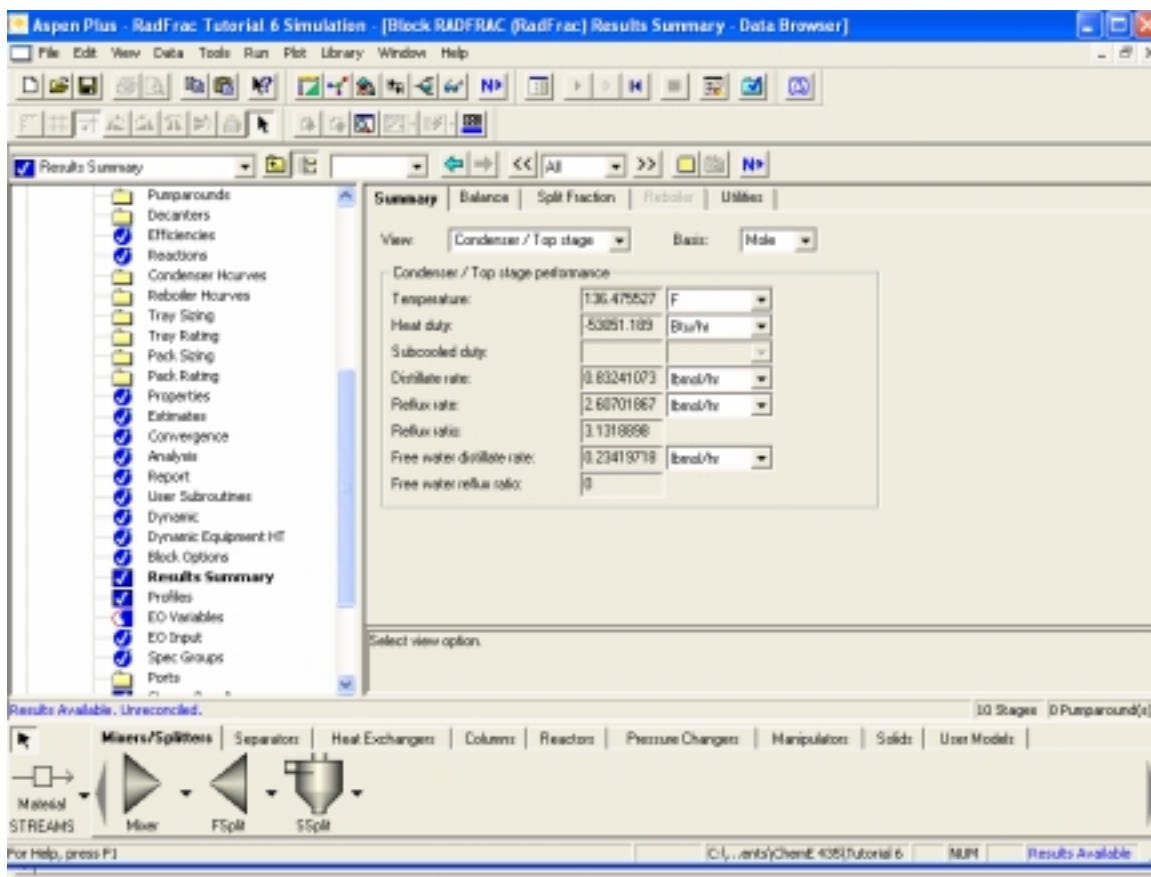
Figure 11: RadFrac Results Summary

This window shows the final operating conditions for the distillation column that were calculated by the program. You can see in this window that our final molar reflux ratio was 3.13. You can also see the required condenser cooling duty. If you switch to the Reboiler / Bottom stage option you can see the required heat input into this column as well.

If you select the Balance tab at the top of the screen, you can see the overall heat and material balances for the column. You can also see the relative difference in the values (emphasizing the fact that no simulation is "perfect").

Under the Profiles option (in the Data Browser options) Aspen presents you with a summary of the operating conditions for this simulation. Under the TPFQ option you can see a breakdown of the liquid and vapor flow rates from each tray. You can also modify the table to show the heat balance or temperature profile. Under the Compositions tab at the top of the screen, you can see a profile of each of the components throughout the

column. If all of your checks appear to be acceptable, you have finished your final Aspen tutorial.

Next Week: Stand-alone Aspen Problem

Hints for next week's final Aspen homework problem:

- Use DSTWU to determine the minimum reflux ratio and number of stages. Under View/Reports, you can generate a report for a DSTWU column that shows this information (if the inputs are correct).

- An input reflux ratio of -1 causes Aspen to use the minimum reflux ratio. Any negative number input as a reflux ratio is used as that number times the minimum reflux ratio (i.e. -2 indicates a reflux ratio of $2*R_{min}$).

- Tables in the Data Browser window can be plotted by selecting each column one at a time and then selecting Plot/X-Axis Variable (or Y-Axis Variable). After each axis variable has been selected the graph can be plotted with Plot/Display Plot.

Tutorial #6 Homework and Solution

Question:

Submit a copy of the Input Summary that is generated for your RadFrac distillation simulation and a stream table with the four final product streams only (two water streams, an acetone stream, and an MIBK stream). For help doing this, see Tutorial #2.

Solution:

;Input Summary created by Aspen Plus Rel. 12.1 at 09:37:13 Tue Nov 16, 2004
;Directory   Filename C:\DOCUME~1\Matt\LOCALS~1\Temp\~ap1a.tmp

TITLE 'Tutorial 6 - RadFrac Distillation'

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

DESCRIPTION "THIS IS THE SOLUTION, DO NOT USE ME"
    General Simulation with English Units :
    F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.

    Property Method: None

    Flow basis for input: Mole

    Stream report composition: Mole flow
    "

DATABANKS PURE12 / AQUEOUS / SOLIDS / INORGANIC / &
        NOASPENPCD

PROP-SOURCES PURE12 / AQUEOUS / SOLIDS / INORGANIC

COMPONENTS
    WATER H2O /
    ACETONE C3H6O-1 /
    METHY-01 C6H12O-2

SOLVE
    PARAM METHOD=EO

FLOWSHEET
    BLOCK MIXER1 IN=FEED MIBK1 OUT=PRODUCT1
    BLOCK FLASH1 IN=PRODUCT1 OUT=VAPPROD1 M-A1 W-A1
    BLOCK MIXER2 IN=W-A1 MIBK2 OUT=PRODUCT2

BLOCK FLASH2 IN=PRODUCT2 OUT=VAPPROD2 M-A2 WATER
BLOCK MIXER3 IN=M-A1 M-A2 OUT=DISTILL
BLOCK RADFRAC IN=DISTILL OUT=ACETONE MIBK FREEWAT

PROPERTIES NRTL

PROP-DATA NRTL-1
  IN-UNITS ENG
  PROP-LIST NRTL
  BPVAL WATER ACETONE .0544000000 755.9488740 .3000000000 0.0 &
      0.0 0.0 68.00000346 203.1800024
  BPVAL ACETONE WATER 6.398100000 -3256.183774 .3000000000 &
      0.0 0.0 0.0 68.00000346 203.1800024
  BPVAL WATER METHY-01 9.162943000 -2247.739182 .2000000000 &
      0.0 0.0 0.0 32.00000374 240.8000021
  BPVAL METHY-01 WATER -3.230481000 2175.978583 .2000000000 &
      0.0 0.0 0.0 32.00000374 240.8000021
  BPVAL ACETONE METHY-01 -5.445200000 3300.340834 .3000000000 &
      0.0 0.0 0.0 77.00000338 230.2340022
  BPVAL METHY-01 ACETONE 5.301300000 -3124.634735 .3000000000 &
      0.0 0.0 0.0 77.00000338 230.2340022

STREAM FEED
  SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=100.
  MASS-FRAC WATER 0.5 / ACETONE 0.5 / METHY-01 0.

STREAM MIBK1
  SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=100.
  MASS-FRAC METHY-01 1.

STREAM MIBK2
  SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=50.
  MASS-FRAC METHY-01 1.

BLOCK MIXER1 MIXER
  PARAM NPHASE=1 PHASE=L
  BLOCK-OPTION FREE-WATER=NO

BLOCK MIXER2 MIXER
  PARAM PRES=50. T-EST=75.

BLOCK MIXER3 MIXER

BLOCK FLASH1 FLASH3
  PARAM TEMP=75. PRES=50.

```
BLOCK FLASH2 FLASH3
   PARAM TEMP=75. PRES=50.

BLOCK RADFRAC RADFRAC
   PARAM NSTAGE=10 NPHASE=2
   COL-CONFIG CONDENSER=TOTAL
   FEEDS DISTILL 5
   PRODUCTS ACETONE 1 L1 / FREEWAT 1 W / MIBK 10 L
   P-SPEC 1 15.
   COL-SPECS D:F=0.99 RW=0. MOLE-RR=1.5
   DB:F-PARAMS COMPS=ACETONE
   BLOCK-OPTION FREE-WATER=YES

DESIGN-SPEC A-PURITY
   DEFINE ACETON MASS-FRAC STREAM=ACETONE SUBSTREAM=MIXED  &
      COMPONENT=ACETONE
   SPEC "ACETON" TO "0.90"
   TOL-SPEC "0.005"
   VARY BLOCK-VAR BLOCK=RADFRAC VARIABLE=MOLE-RR  &
      SENTENCE=COL-SPECS
   LIMITS "0.5" "5.0"

DESIGN-SPEC W-PURITY
   DEFINE WATER MASS-FRAC STREAM=WATER SUBSTREAM=MIXED  &
      COMPONENT=WATER
   SPEC "WATER" TO "0.95"
   TOL-SPEC "0.001"
   VARY MASS-FLOW STREAM=MIBK2 SUBSTREAM=MIXED  &
      COMPONENT=METHY-01
   LIMITS "25" "400"

EO-CONV-OPTI

STREAM-REPOR WIDE NOMOLEFLOW MASSFLOW MASSFRAC
;
```

Aspen Tutorial #6

Tutorial 6 - RadFrac Distillation					
Stream ID		WATER	FREEWAT	ACETONE	MIBK
Temperature	F	75.0	136.5	136.5	208.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	2.100	0.234	0.832	4.707
Mass Flow	lb/hr	39.294	4.219	45.126	435.837
Volume Flow	cuft/hr	0.641	0.069	0.954	9.532
Enthalpy	MMBtu/hr	-0.258	-0.029	-0.090	-0.618
Mass Flow	lb/hr				
WATER		37.334	4.219	1.938	6.509
ACETONE		1.165		40.596	8.239
METHY-01		0.795		2.592	421.089
Mass Frac					
WATER		0.950	1.000	0.043	0.015
ACETONE		0.030		0.900	0.019
METHY-01		0.020		0.057	0.966