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Disclaimer: This document is based on the Mario Richard Eden's Aspen Simulation document for Auburn University. We would like to thank Dr. Eden for allowing us to use his information.

Introduction to Aspen Plus Simulation

What is Process Simulation/Analysis?

The purpose of analysis/simulation is to model and predict the performance of a process. It involves the decomposition of the process into its constituent elements (e.g. units) for individual study of performance. The process characteristics (e.g. flowrates, compositions, temperatures, pressures, properties, equipment sizes, etc.) are predicted using analysis techniques. These techniques include mathematical models, empirical correlations and computer-aided process simulation tools (e. g. ASPEN Plus). In addition, process analysis may involve the use of experimental means to predict and validate performance. Therefore, in process simulation, we are given the process inputs and flowsheet and are required to predict process outputs (Figure 1). The lab will focus on ASPEN Plus. It is a computer-aided software which uses the underlying physical relationships (e.g. material and energy balances, thermodynamic equilibrium, rate equations) to predict process performance (e.g. stream properties, operating conditions, and equipment sizes).

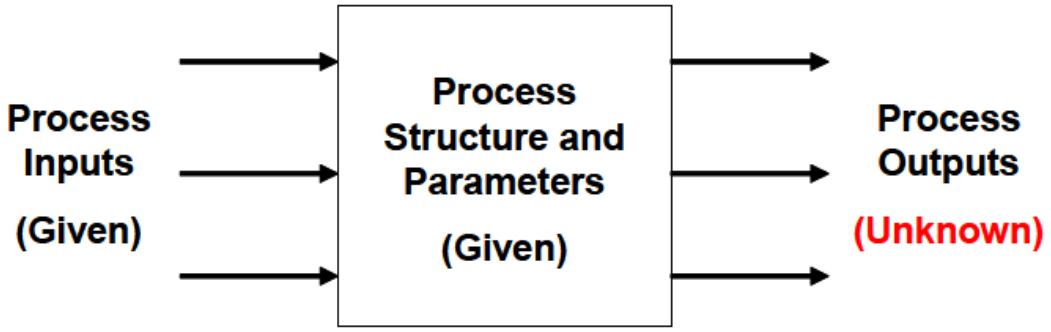

Figure 1. Process simulation problems

There are several advantages of computer-aided simulation:

- Allows the designer to quickly test the performance of synthesized process flowsheets and provide feedback to the process synthesis activities
- Can be coordinated with process synthesis to develop optimum integrated designs.
- Minimizes experimental and scale-up efforts
- Explores process flexibility and sensitivity by answering "what if" questions
- Quantitatively models the process and sheds insights on process performance

Important issues to remember before venturing in to the exciting world of computer-aided simulation:

- Do NOT implicitly trust the results of ANY simulation tool
- The calculated results are only as good as the input you give the simulator
- ALWAYS convince yourself that the obtained results make physical sense, otherwise you will NEVER be able to convince someone else of the merits of your work

Basic Information on ASPEN PLUS and Its Graphical Operations

I. How do I start it?

From the windows start menu, select All Programs then AspenTech. Now select Process Modeling V8.4 then Aspen Plus. Select Aspen Plus V8.4 (Fig 2)

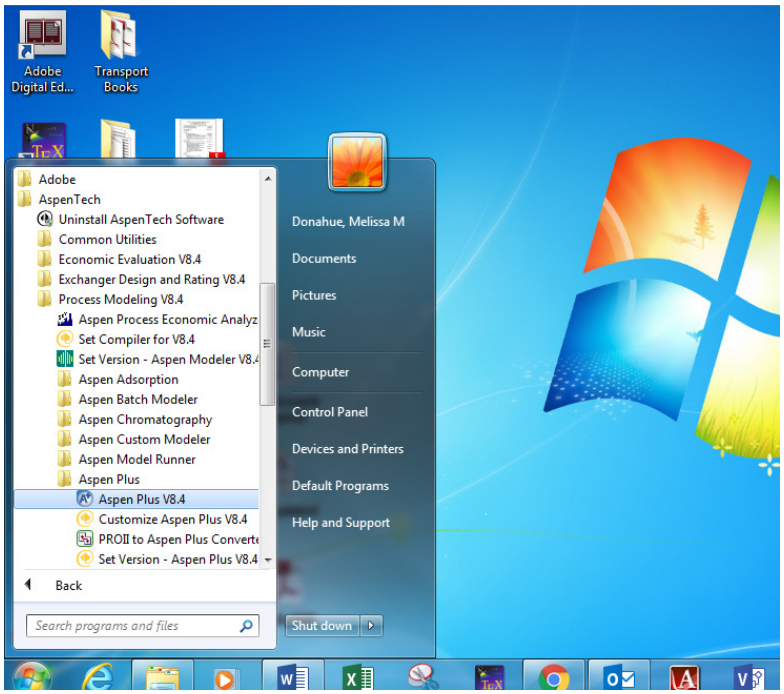

Figure 2. Starting Aspen Plus

Next you will have the option of opening an existing file or starting a new simulation. Choose a new simulation and select blank simulation (Fig 3). Notice that you have the option of using existing templates.

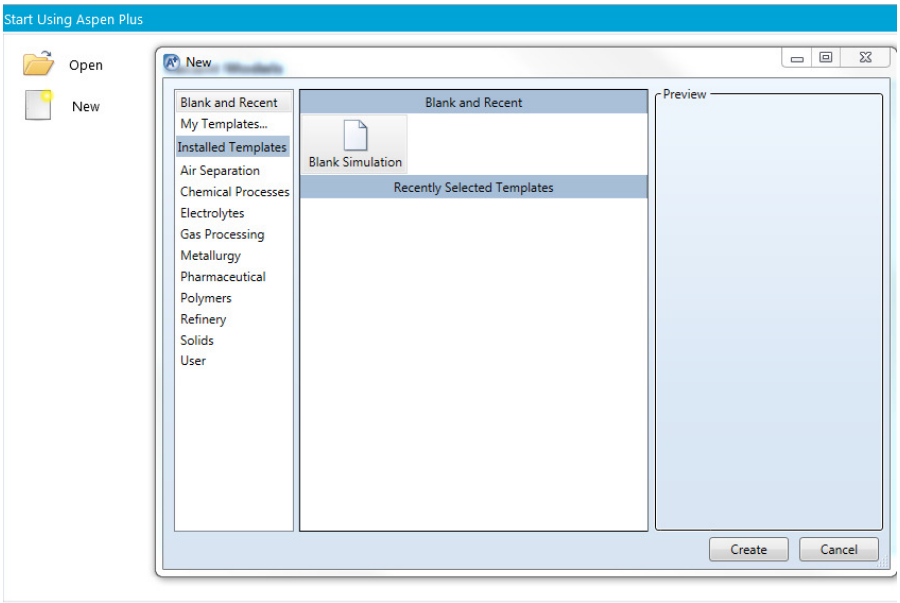

Figure 3. Starting a Simulation

ASPEN Plus will display the User Interface (Fig 4). Features of the User Interface include:

- Quick Access Toolbar allows direct access to commonly-used functions
- Ribbons display the most commonly used commands
- Environment Buttons allows navigation between properties, simulation, and energy analysis
- Window Tabs appear for each form that is open. Clicking on a tab will make that form the active window
- Navigation pane is used to navigate folders, forms, and sheets
- Sheets make up forms and forms make up folders (a sheet in a form in a folder)
- Folders are the root items n the Data Browser
- Forms are located in folders and are used to enter data and view simulation results
- Sheets are contained in folders and are selected using tabs at the top of each sheet

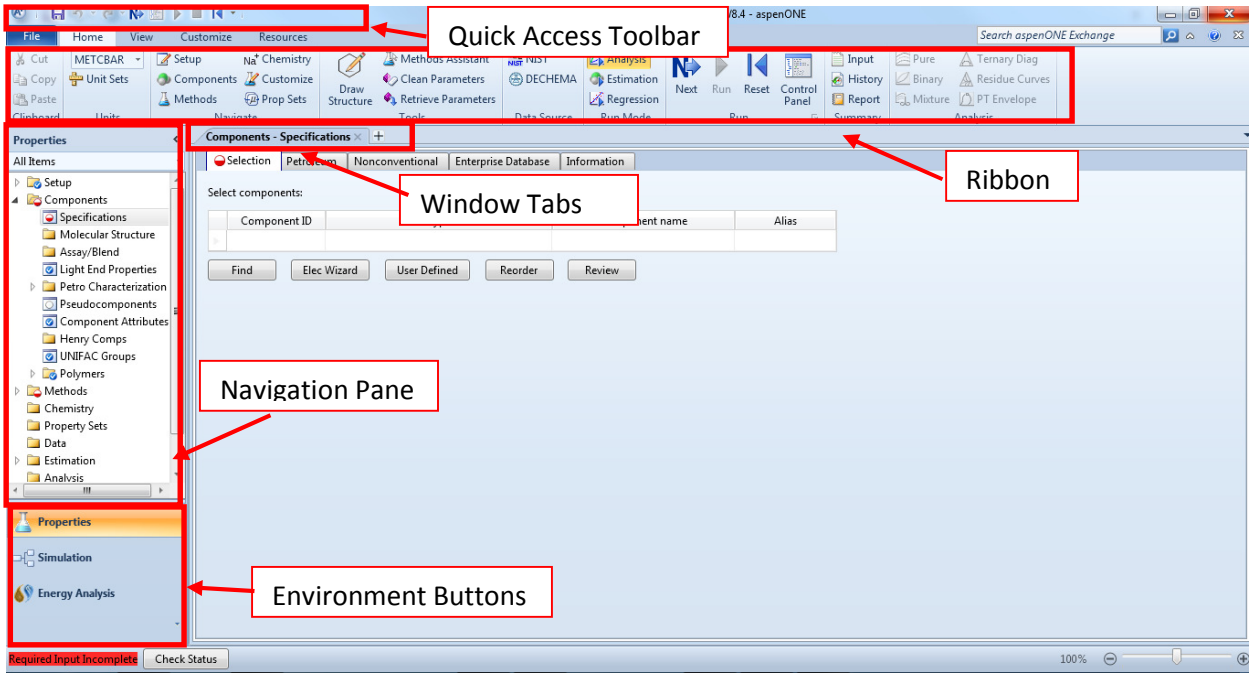

Figure 4. Aspen Plus V8.4 User Interface

II. Mouse Functions:

- Left Button Click: select object/field
- Right Button Click: Bring a menu for a selected object/field
- Double Left Click: Open Navigation Pane object sheet

III. How to Start a Simulation

Before drawing your flowsheet, you must specify the components in the model and set the calculation methods for physical properties. Both of these are done in the Properties Environment.

To add a component, click on the Components folder and click the Find button. A dialogue box will appear where you can enter your desired component. Aspen will generate a list of compound matching

your search criterion (Figure 5). To add a component, highlight it in the list and click “Add selected compounds”.

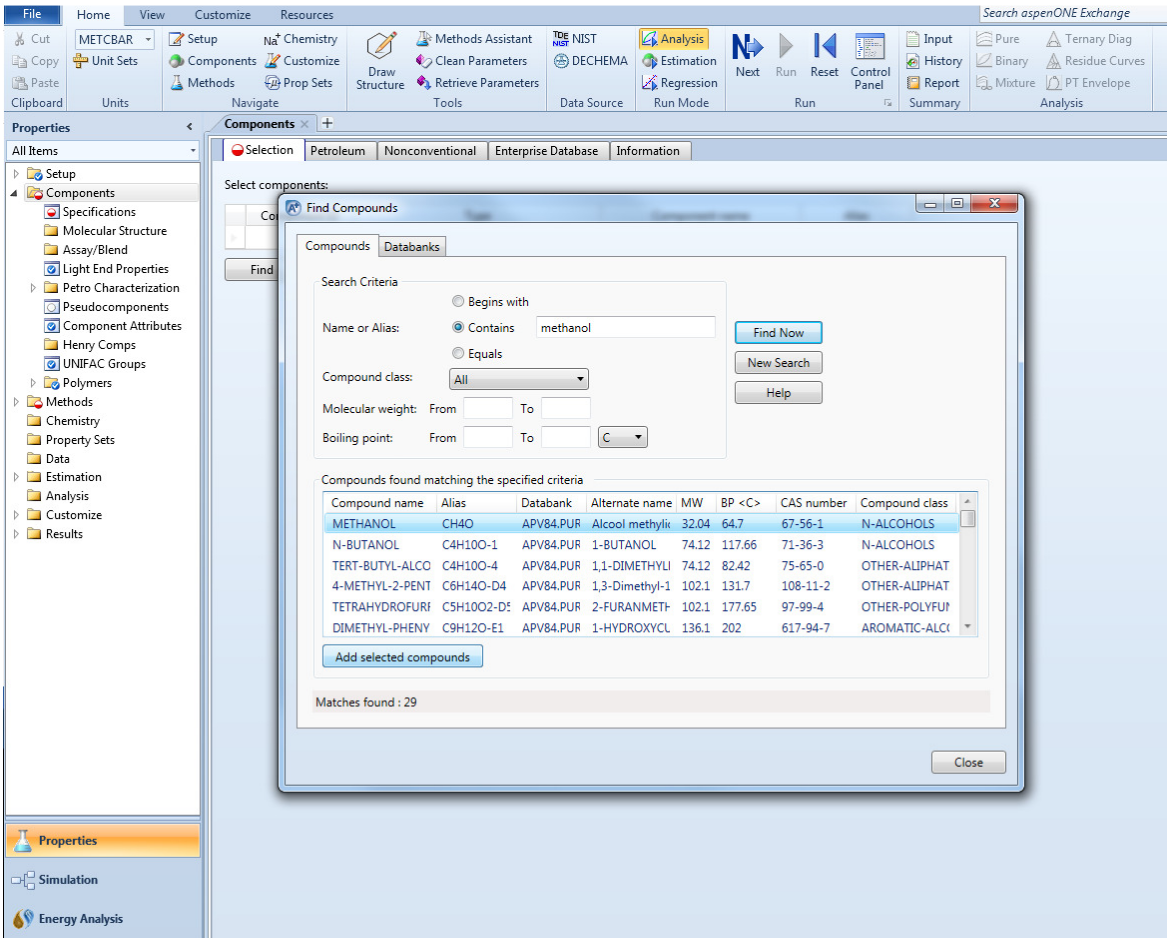

Figure 5. Adding Components in Aspen

To select a property method for your simulation, click on the Methods folder. Click on the Method filter dropdown to choose a process type, and click on the Base method dropdown to choose a property method (Figure 6). Conversely, you can also choose from the Method Name dropdown which displays all the available property methods.

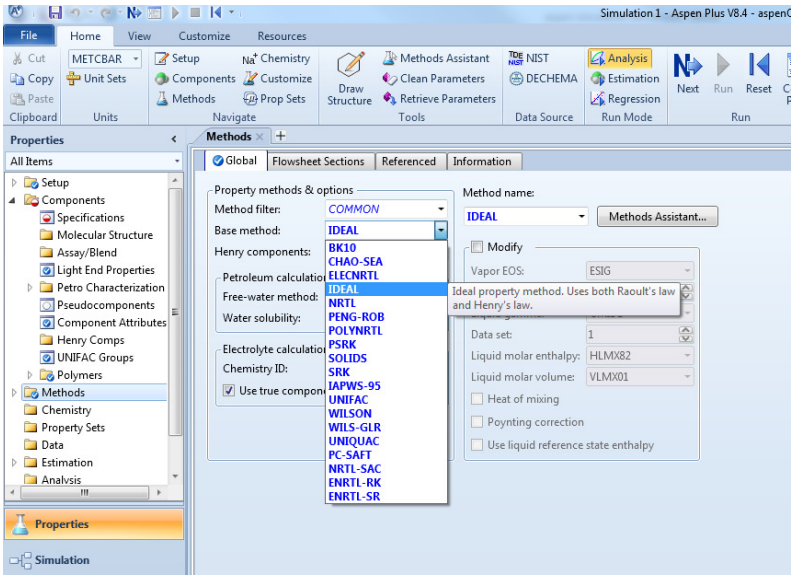

Figure 6. Selecting a Property Method in Aspen

IV. How to Draw a Flowsheet

A flowsheet consists of blocks connected with streams. In order to place a block:

- Go to the Simulation environment. The Model Palette should appear at the bottom of the screen
- Click (left button click) on a model category tab in the Model Palette
- Click on a unit operation in the Model Palette. Click (left) on the drop-down arrow to how you want to draw the unit. Click (left) on the icon and drag it onto the Process Flowsheet Window
- If instead of dragging the icon, you click on it you will see the + sign when you move to the Process Flowsheet Window. This signals that you are in a multiple entry mode. In this case each time you click (left), you will repeatedly placing the block. To stop placing blocks, click (right mouse button) anywhere in the Process Flowsheet Window or click (left mouse button) on the mouse button in the top left of the Model Palette.

As an illustration, suppose we would like to draw a compressor. First, we click, on the Pressure Changers unit operation model, then we click on the compressor block, then we click on the drop-down arrow to choose an icon for the compressor (Fig. 7).

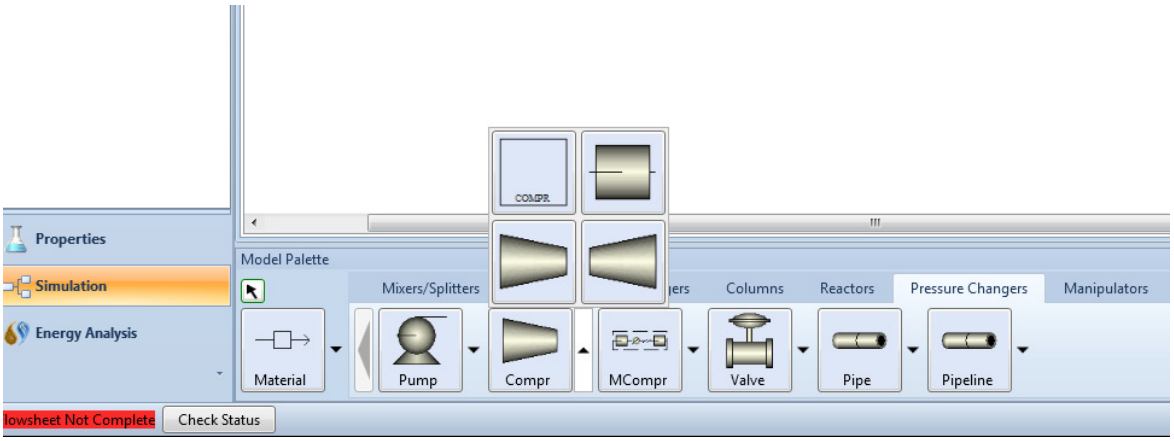

Figure 7. Selecting an icon for a Compressor

To add a material stream, click on the Material block and place the cursor above the desired unit operation. When you do this, red and blue arrows will appear on your unit operations. The red arrows represent required input/outputs, and the blue arrows represent optional inputs/outputs (Figure 8).

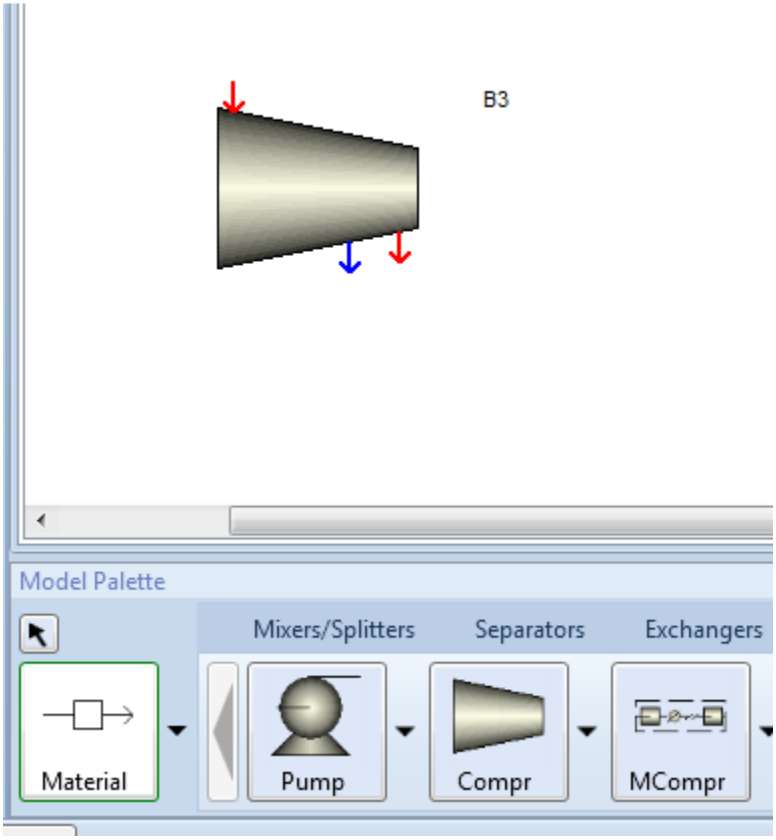

Figure 8. Adding material streams to blocks

IV. Useful Symbols

Figure 9 illustrates some of the symbols that are commonly used in Aspen Plus

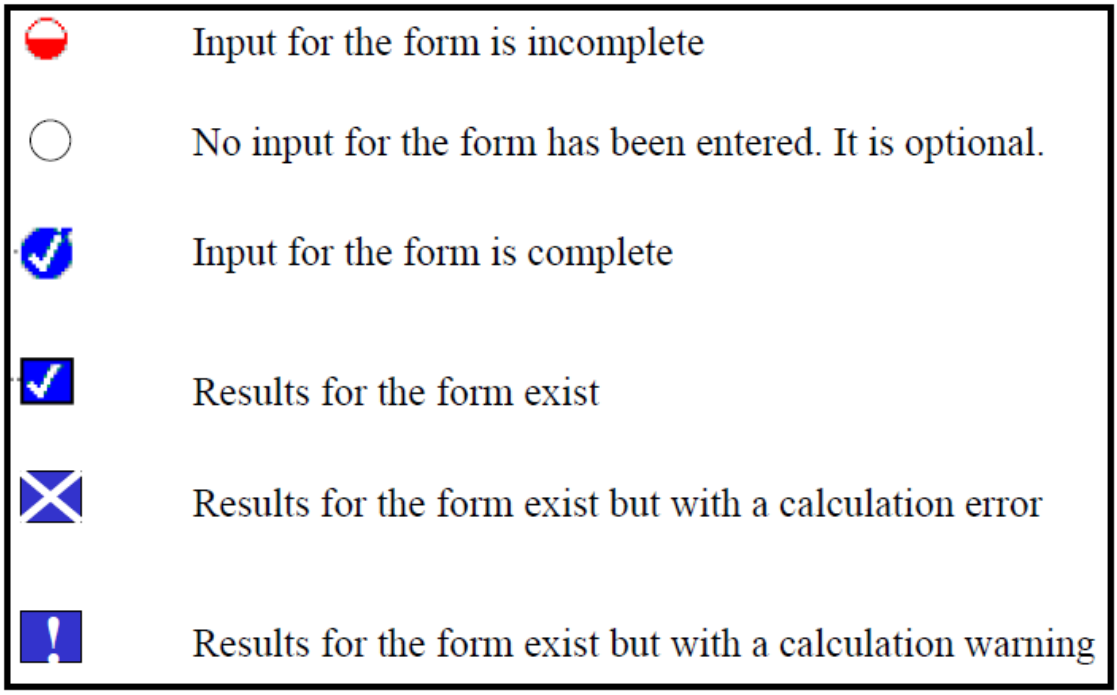

Figure 9. Useful Symbols

V. The Navigation Pane

The Navigation Pane is a sheet and form viewer with a hierarchical tree view of the available simulation input, results, and objects that have been defined.

Use the Navigation Pane to:

- Display forms and sheets and manipulate objects
- Edit the sheets that define the input for the flowsheet simulation
- Check the status and contents of a run
- See what results are available

VI. Main Data

In addition to drawing the flowsheet, you need to provide data for the main folders:

1. Setup: this folder is used to specify information on the simulation, units, etc.
2. Stream: this folder is where you enter stream data
3. Blocks: folder for providing data on the process equipment

Formatting and Generating Reports

As the workshops become increasingly more difficult it will become important to be able to get your results. Aspen allows you to print off reports of many different aspects of your flowsheet: streams, convergences, units, etc. The default text editor used in Aspen is Notepad. This tutorial will show you how to change your text editor to Microsoft Word and how to generate reports with Word. It will also show you how to place the stream data on your flowsheet.

Changing Text Editors

To change your text editor begin by opening Aspen Plus User Interface. Then, select *blank simulation* at the startup menu. Once in the Aspen Plus window, click on *File*, and then select *Options*. This will bring up the options window. From the options window, select the *Advanced* tab. Under *Text file settings,* you will see that text editor has Notepad in the white box next to it. One option is to use the *Browse* button to find word yourself. Alternatively, you can click on the white box, delete notepad, and type in C:\Program\Fiels\MicrosoftOffice\Office\Winword.exe or something similar depending on your computer configuration. This will change the text editor to Microsoft Word instead of notepad.. Then, click *OK* at the bottom of the Options window.

Generating Reports

After completing a simulation in Aspen, you can get the result of various items (streams, units, etc.) by using the report feature. After completing a simulation, go to the *Home* tab and select *Report* from the Summary group in the ribbon. This will open the report window. The report window has a *Display report for* block with a drop down arrow. If you click on the drop down arrow, you will see many options. The two significant items are *Streams* and *Blocks*. If you select *Blocks* from the drop down arrow, you will notice that all the blocks in your process appear in the large white space labeled *Block IDs* (you may need to expand a *Select All* folder). The blocks are the units in your process. By selecting a block, for example, B1 and clicking *OK,* Microsoft Word will open up and display the results for that unit. When Word opens, there may be a file conversion window that appears. If this happens, just click *OK* and your results should appear. Similarly, had you selected *Streams* from the drop down menu and selected one in the ID box, you could have displayed the results of a stream.

Adding Stream Data to your Flowsheet

In some cases it may be advantageous to place your stream data on the process flowsheet. After running a simulation, click on the Navigation Pane. Click on the *Results Summary* folder and then on *Streams*. This will bring up the results of your stream data. On this window, there will be a button labeled *Stream Table*; by selecting this button you will place the stream results in your process flowsheet. You could have also placed the results of each stream in separately by going to the *Streams* folder and selecting individual streams and their results.

Report Properties

As discussed earlier, Aspen Plus can generate reports within a text editor that contain information regarding a simulation. By default, Aspen provides stream flowrates, temperatures, and various other data. However, information, such as the mole fraction of a component within a stream, is often desired but no provide by default. Therefore, it is necessary to customize your report properties within Aspen so

that the information you desire is generated directly from Aspen instead of by hand or from a secondary program such as Excel. To customize the report properties within Aspen, first go in to the Navigation Pane, then click the *Setup* folder and then click *Report Options*. This can be seen below in Figure 10. The report options displays six tabs (General, Flowsheet, Block, Stream, Property, and ADA). These tabs allow you to browse the specified areas and customize what information is generated within reports. The *Stream* tab is of particular importance because it allows the selection of both the flow and fraction basis within the report, also seen below in Figure 10. It is important to note that the report options must be specified prior to running the simulation. Otherwise, the desired information will not be generated.

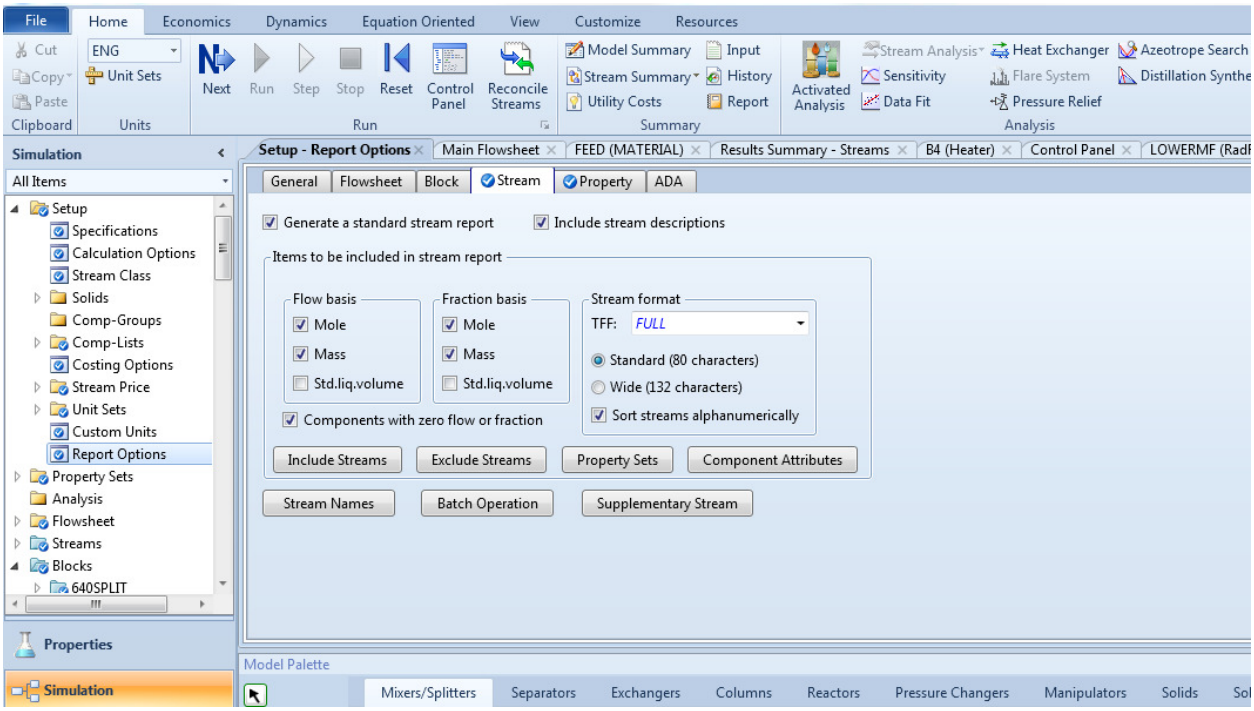

Figure 10. Report Options

Additionally, when running a simulation the question may arise as to how Aspen is determining the heat capacity, or a similar property, of the chemicals within the simulation. Within the *Report Options* category, Aspen allows the user to request that property estimation information be provided. To do this, check the *Property* tab within *Report Options* (Figure 11). Under the title “Items to be included in report file” there are four check boxes that allow the user to specify the information he/she want to be generated within a report.

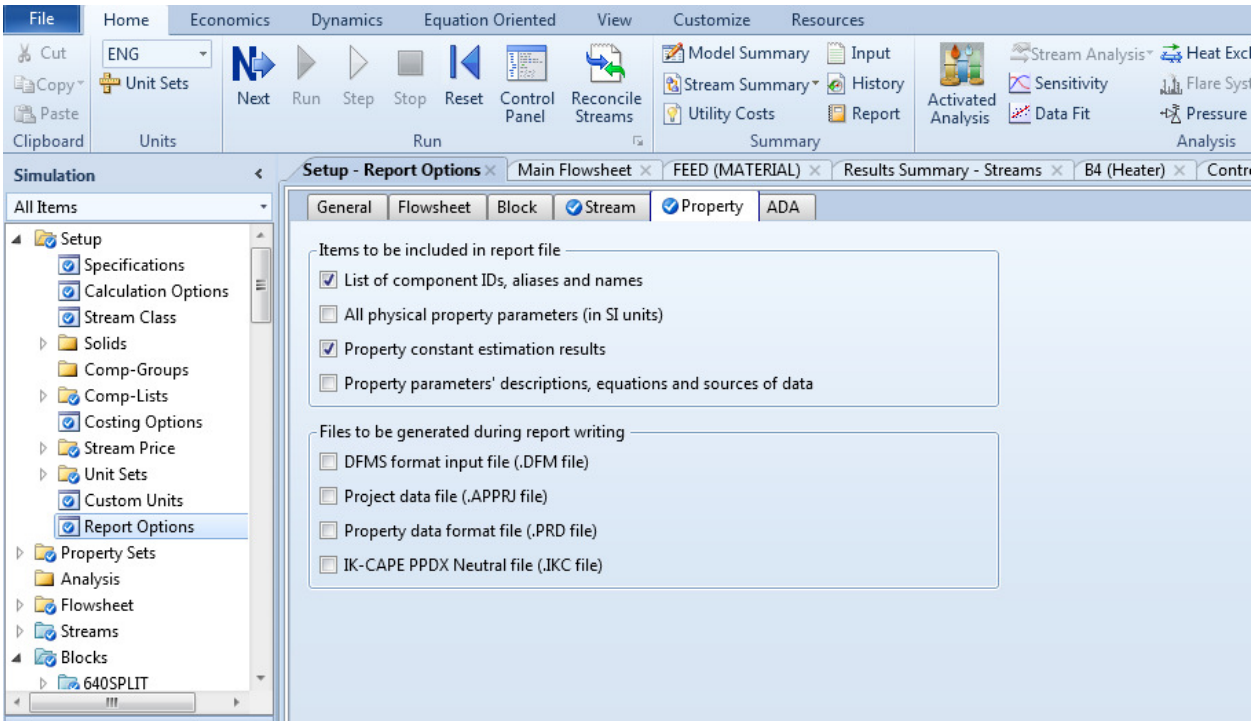

Figure 11. Property Estimation Options

After selecting the desired property information within the Report Options, the user proceeds to fill out the required information within the Navigation Pane and then runs the simulation. Specified properties such as mole fraction will appear in both the results folder and within a report generated for a block or a stream (report generation has been discussed earlier). However, the property estimation information will not appear in either location. To obtain this information, the user must generate a report for the simulation. To do this, go to *Report* as you did for generating a stream or block report. A window will appear with a drop down box. Scroll through the options until *Simulation* appears. Select *simulation* and then click *OK*. This will generate a report containing all the property estimation information selected previously.

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PHYSICAL PROPERTIES AND SELECTION OF THERMODYNAMIC MODELS

A property method is a collection of equations used to calculate all physical properties. Each property method contains a specific equation to calculate a given property, such as enthalpy, density, etc. ASPEN Plus contains several property methods. How do you choose an appropriate method? This is the focus of this tutorial.

The key thermodynamic property calculations performed in a simulation is phase equilibrium. The basic relationship for every component i in the vapor and liquid phases of a system at equilibrium is that fugacity in the liquid phase = fugacity in the vapor phase. What is fugacity??? (Here we go, past courses coming back to haunt you ☺). ***Fugacity*** is a measure of the tendency of a component of a liquid mixture to escape, or vaporize, from the mixture. The composition of the vapor form of the mixture, above the liquid, is not the same as that of the liquid mixture; it is richer in the molecules of that component that has a greater tendency to escape from the liquid phase. The fugacity of a pure component f_i^0 is related to the pressure that it exerts in the vapor phase through a fugacity coefficient (ϕ_i^o):

$$f_i^0 = \phi_i^o P$$

In an ideal gas, $\phi_i^o = 1$ and the fugacity is equal to the pressure. When we have mixtures, fugacity of component I in the mixture is related to the pure-component fugacity by:

$f_i^v = y_i f_{i,v}{}^0$ for the vapor and,

$f_i^L = x_i f_{i,L}{}^0$ for the liquid (where y and x represent mole fractions in the vapor and liquid phases).

Hence, $f_i^v = \phi_{i,v}\, y_i P$ and $f_i^L = \phi_{i,L}\, x_i P$. At equilibrium, both fugacities should be equal.

Fugacities can be calculated using two main methods: *equations of state, activity coefficient models, ideal systems, and special models*. Let us review all of them.

EQUATIONS OF STATE

Classical thermodynamics provides a means for properties such as enthalpies and densities from P-V-T relations which are referred to as the Equations of State (EOS). Some of the common EOS include cubic equations of state and the virial equations of state. Steam tables are an example of another type of

equation of state. The simplest equation of state is the ideal gas law (PV = nRT). The ideal gas law assumes that molecules have no size and that there are no intermolecular interactions. This can be called absolute ideality, in contrast to ideality defined relative to pure component behavior, as used in the activity coefficient approach. Examples of **EOS Models** for predicting properties include:

- **Redlich-Kwong-Soave**
- **Redlich-Kwong**
- **Peng Robinson**
- **Sanchez-Lacombe (for polymers)**

> *With an equation-of-state method, all properties can be derived from the equation of state, for both phases.*

ACTIVITY COEFFICIENT MODELS

At a given temperature, the ratio of a fugacity of a component in the mixture to its fugacity in some standard state (e.g., fugacity of pure component) is termed activity, a. Hence,

$$a_i = \frac{f_i}{f_i^o}$$

The activity is related to mole fractions via the activity coefficient γ as follows:

$a_{i,v} = \gamma_{i,v} y_i$ and $a_{i,L} = \gamma_{i,L} x_i$

For ideal solutions: $\gamma_{i,v} = \gamma_{i,L} = 1.0$

In non-ideal solutions, the activity coefficient is estimated through a variety of models. Examples of **activity coefficient models** include:

- **Wilson**
- **Van Laar**
- **UNIFAC**
- **UNIQUAC**
- **Flory Huggins**
- **NRTL**
- **Electrolyte NRTL**
- **Scatchard Hildebrand**

The activity coefficient represents the deviation of the mixture from ideality (as defined by the ideal solution). The greater the deviation from unity, the more non-ideal the mixture is. In the majority of mixtures, the activity coefficient is greater than unity. The result is a higher fugacity than ideal. As mentioned earlier, the fugacity can be interpreted as the tendency to vaporize. If compounds vaporize more than in an ideal solution, then they increase their average distance. So activity coefficients greater than unity indicate repulsion between unlike molecules. If the repulsion is strong, liquid-liquid separation occurs. This is another mechanism that decreases close contact between unlike molecules. It

is less common that the activity coefficient is smaller than unity. Using the same reasoning, this can be interpreted as strong attraction between unlike molecules. In this case, liquid-liquid separation does not occur. Instead formation of complexes is possible.

> *Using an activity coeffici ent method, the vapor phas e properties are derived from an equation of state, exactly as in the equation-of- state method. However the liquid properties are determined from summation of the pure component properties to which a mixing term or an excess term is added.*

IDEAL MODELS

An ideal system is one that follows the ideal gas law (PV=nRT) in the vapor phase and Raoult's law in the liquid phase. Ideal gas law is typically acceptable at low pressures. The ideal solution assumes that all molecules in the liquid solution are identical in size and are randomly distributed. This assumption is valid for mixtures containing molecules of similar size and character. Ideality can also exist between polar molecules, if the interactions cancel out.

In general, you can expect non-ideality in mixtures of unlike molecules or when you have polar components. An example of a strong polar compound is water. The following is a list of relative polarities of functional groups starting with the most polar and ending with least polar:

1. Water
2. Organic acids
3. Amines
4. Alcohols
5. Esters
6. Ketones
7. Aldehydes
8. Ethers
9. Aromatics
10. Olefins
11. Paraffins

Either the size and shape or the intermolecular interactions between components may be dissimilar. For short these are called size and energy asymmetry. Energy asymmetry occurs between polar and non-polar molecules and also between different polar molecules. An example is a mixture of alcohol and water.

The IDEAL property method accommodates both Raoult's law and Henry's law. This method employs the following relationships and correlations:

- Ideal activity coefficient model for the liquid phase (activity coefficient = 1)
- Ideal gas equation of state for the vapor phase (PV = nRT)
- Ideal mixing in liquid

SPECIAL MODELS

For specific systems, there are special models that can be used to predict properties. Examples of such special models include:

- Steam Tables
- API Sour-Water Method
- Kent-Eisenberg

USE OF HENRY'S LAW

Henry's law is only used with ideal and activity-coefficient models. It is used to determine the amount of a supercritical component or a light (non-condensable) gas (e.g., CO_2, N_2, etc.) in the liquid phase. To use Henry's law for non-condensable components, you must designate these components as Henry's components on the Components Henry-Comps form. Henry's constant model parameters (HENRY) must be available for the solute with at least one solvent. Use the Properties Parameters Binary Interaction form (HENRY-1) to enter Henry's constants or to review built-in parameters. ASPEN Plus contains an extensive collection of Henry's constants for many solutes in solvents. Solvents are water and other organic components. ASPEN Plus uses these parameters automatically when you specify the IDEAL property method.

If you are doubtful about the ideality of a system, you can develop Y-X or T-Y-X plot to examine the behavior of the mixture.

ROADMAP FOR CHOOSING A PROPERTY METHOD

In most cases, the comparison will be between the use of wither EOS models or activity coefficient models. The following table describes some of the key features for each.

TABLE 1. Comparison Between EOS and Activity Coefficient Models

EOS Models	Activity Coefficient Models
Limited in ability to represent non-ideal liquids	Can represent highly non-ideal liquids
Consistent in critical region	Inconsistent in critical region
Can represent both the vapor and liquid phases	Can represent the liquid phase only. Therefore, the gas phase must still be described by an EOS model
Parameters extrapolate well with temperature	Binary parameters are highly dependent on temperature

If you don't have an exact model for your system, you may use the following tree search to select the thermodynamic model.

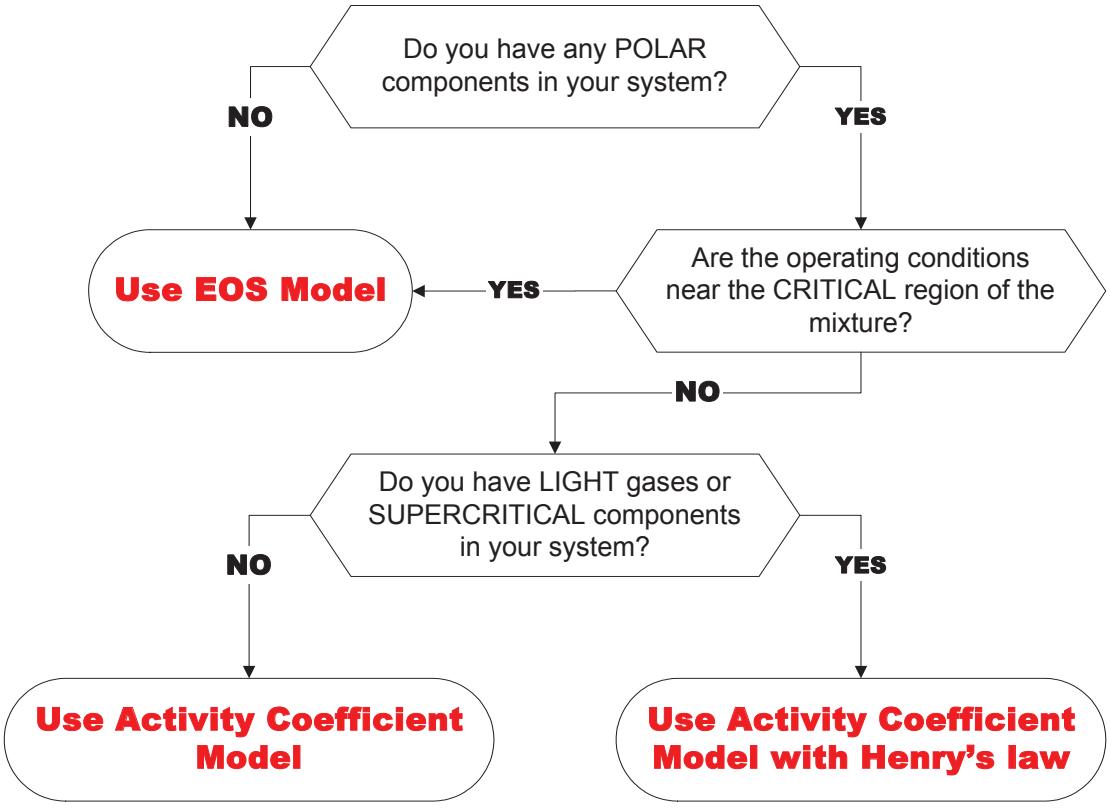


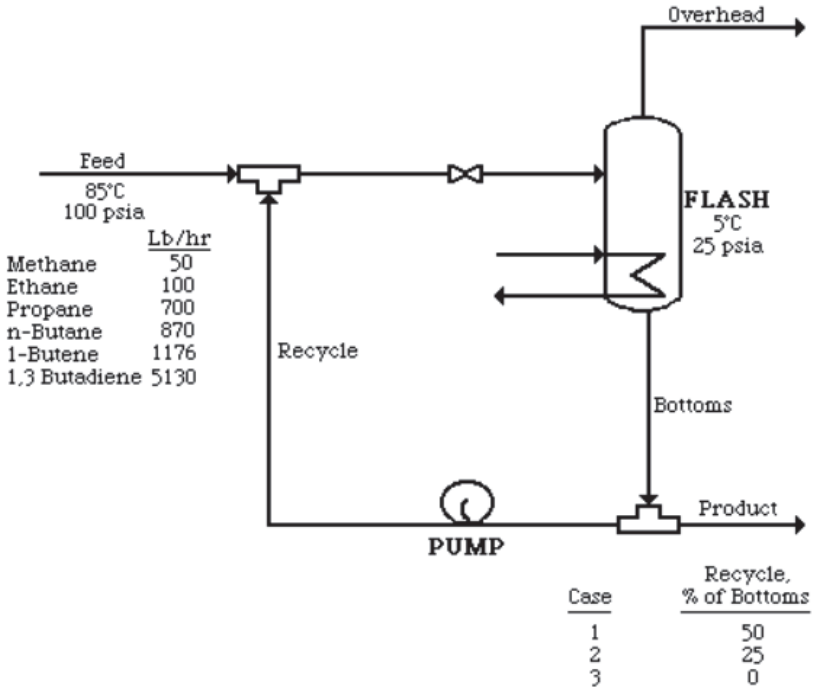
Fig. 1. Tree Search for Selection of Thermodynamic Model

TABLE 2. Recommended Models for Sample Systems

System	Ideality Issues	Recommended Model
Water-Benzene	Water is polar	Activity coefficient model
Propane-Ethane-Butane	No polarity	Equation of state (EOS)
Benzene-Toluene	No polarity, but similar sizes	Equation of state (EOS)
Water-Ethanol	Water is polar	Activity coefficient model
Acetone-Water-Carbon Dioxide	Presence of light gases	Activity coefficient model with CO2 designated as Henry's compound

Exercise A.1 Flash with Recycle Problem (Exercise 3.1, SSL)

a. Consider the flash separation process shown below:



If using ASPEN PLUS, solve all three cases using the MIXER, FLASH2, FSPLIT, and PUMP subroutines and the RK-SOAVE option set for thermophysical properties. Compare and discuss the flow rates and compositions for the overhead stream produced by each of the three cases.

b. Modify Case 3 of Exercise 3.1a to determine the flash temperature necessary to obtain 850 lb/hr of overhead vapor. If using ASPEN PLUS, a design specification can be used to adjust the temperature of the flash drum to obtain the desired overhead flow rate.

ASPEN PLUS Solution

Exercise B.1 Refrigerator Design Problem

This is extension of Example 6.2 in Seider, Seader, and Lewin (1999), which involves a refrigeration loop:

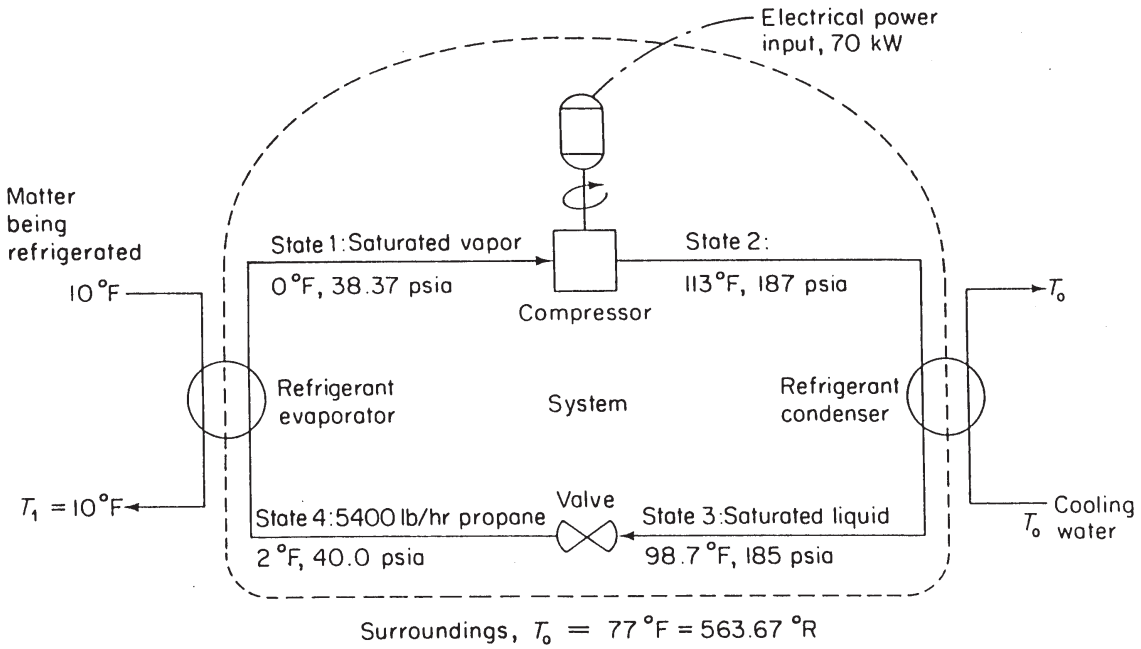


Figure 6.9 Operating Conditions for Propane Refrigeration Cycle

In this problem, it is desired to:

a. simulate the refrigeration cycle assuming that the compressor has an isentropic efficiency of 0.9. For the evaporator and condenser, do not simulate the heat exchangers. Instead, use models that compute the "heat required" to be absorbed by the evaporating propane and to be removed from the condensing propane. Use the Soave-Redlich-Kwong equation and a propane flow rate of 5,400 lb/hr. Set the pressure levels as indicated above, but recognize that the temperatures may differ due to the VLE model.

b. calculate the lost work and the thermodynamic efficiency for the refrigeration cycle.

HYSYS.Plant Solution	ASPEN PLUS Solution

Exercise B.2 VLLE Problem

An equimolar stream of benzene, toluene, and water at 150 kgmole/hr, 100°C, and 7 bar enters a flash vessel. It is expanded to 0.5 bar and cooled to 60°C. Use a process simulator with the UNIFAC method, having liquid-liquid interaction coefficients, for estimating liquid-phase activity coefficients to compute the flow rates and compositions of the three product streams. Also, determine the heat added or removed. If using ASPEN PLUS, the FLASH3 subroutine and the UNIF-LL property option are appropriate. If using HYSYS.Plant, use the **3-phase Separator**, and select the appropriate physical property method as guided by the **multimedia**.

HYSYS.Plant Solution	ASPEN PLUS Solution

Exercise B.3 VLE Data Regression Problem

The following vapor-liquid equilibrium data for ethanol and benzene at 1 atm have been taken from the Gmehling and Onken data bank:

x	y	T,°C
0	0	80.13
0.025	0.1303	76.29
0.05	0.2117	73.77
0.075	0.2654	72.09
0.1	0.3029	70.94
0.125	0.3304	70.12
0.15	0.3514	69.53
0.175	0.3681	69.08
0.2	0.3818	68.75
0.225	0.3933	68.49
0.25	0.4033	68.28
0.275	0.4121	68.12
0.3	0.4201	68.00
0.325	0.4274	67.90
0.35	0.4343	67.82
0.375	0.4408	67.76
0.4	0.4472	67.72
0.425	0.4534	67.69
0.45	0.4596	67.68
0.475	0.4659	67.68
0.5	0.4724	67.69
0.525	0.4791	67.72
0.55	0.4860	67.77
0.575	0.4935	67.82
0.6	0.5015	67.90
0.625	0.5101	68.00
0.65	0.5195	68.13
0.675	0.5298	68.28
0.7	0.5413	68.47
0.725	0.5542	68.69
0.75	0.5689	68.97
0.775	0.5856	69.30
0.8	0.6049	69.70
0.825	0.6273	70.19
0.85	0.6539	70.78
0.875	0.6855	71.49
0.9	0.7238	72.36
0.925	0.7707	73.41
0.95	0.8293	74.72
0.975	0.9036	76.32
1	1	78.31

For the design of a distillation column to produce nearly pure ethanol, it is desired to obtain a close match between the computed VLE and the Gmehling and Onken data.

a. Use the binary interaction coefficients for the UNIQUAC equation for liquid-phase interaction coefficients, in the data bank of a process simulator, to prepare T-x-y and x-y diagrams.

b. Use data points having ethanol mole fractions above its azeotropic mole fraction with a regression program in a process simulator. Determine interaction coefficients that give better agreement with the Gmehling and Onken data at high ethanol concentrations. Show how the T-x-y and x-y diagrams compare using these data points.

ASPEN PLUS Solution

Exercise B.4 Chemical Equilibrium Problem

An equimolar stream of ammonia, oxygen, nitrogen oxide (NO), nitrogen dioxide (NO_2), and water at 100 lbmole/hr, 300°F, and 1 atm enters a tank reactor. Determine the flow rate and composition of the reactor effluent, assuming that chemical equilibrium is attained. Use a process simulator, assuming that the ideal gas law applies.

a. Determine the number of independent reactions. Then, determine a set of independent reactions.

b. Obtain chemical equilibrium by solving the mass-action equations (using K-values). If using ASPEN PLUS, the REQUIL subroutine is appropriate.

c. Obtain chemical equilibrium by minimizing the Gibbs free energy. Note that it is not necessary to specify an independent reaction set. If using ASPEN PLUS, the RGIBBS subroutine is appropriate.

ASPEN PLUS Solution

Exercise B.5 Selection of an Environmentally-friendly Refrigerant

It is desired to find a refrigerant that removes heat at -20°C and rejects heat at 32°C. Desirable refrigerants should have $P^s\{-20°C\} > 1.4$ bar, $P^s\{32°C\} < 14$ bar, $\Delta H^v\{-20°C\} > 18.4$ kJ/mol, and $c_{pl}\{6°C\} > 18.4$ kJ/mol. For the candidate groups, CH_3, CH, F, and S, formulate a mixed-integer nonlinear program and use GAMS to solve it. Hint: maximize the objective function, $\Delta H^v\{-20°C\}$.

Exercise D.1 Multicomponent Distillation Design Problem 1

In the manufacture of higher alcohols from carbon monoxide and hydrogen, a mixture of alcohols is obtained, which must be separated into desired products. A feed mixture of:

	mol%
ethanol	25
n-propanol	50
iso-butanol	10
n-butanol	15

has been isolated from methanol and heavier alcohols in prior distillation steps. It is a saturated liquid at the pressure of the first distillation column, to be determined in 'a' below.

The three desired products are streams containing:

1. At least 98% of the ethanol at a purity of 98 mol%.

2. N-propanol with essentially all of the remaining ethanol and no more than 2% of the isobutanol in the feed mixture.

3. At least 98% of the iso-butanol, all of the n-butanol, and no more than 1% of the n-propanol, in the feed mixture.

Two distillation towers are used. The first receives the feed mixture. Its distillate is fed to the second tower, which produces ethanol-rich and n-propanol-rich products.

Use a process simulator to:

a. Determine the tower pressures that permit cooling water to be used in the condensers; that is, let the cooling water be heated from 90-120°F and the bubble-point of the condensed overhead vapor be 130°F or higher. This assures that the minimum approach temperature difference is 10°F. Use total condensers. To avoid vacuum operation, pressures in the towers must exceed 20 psia. Assume no pressure drop in the towers. In ASPEN PLUS, use the SEP2 subroutine. In HYSYS.Plant, use **Splitter.**

b. Determine the minimum number of trays and the minimum reflux ratio. Then, let the actual reflux ratio be $1.3 \times R_{min}$ and use the Gilliland correlation to determine the theoretical number of trays and the location of the feed tray. In ASPEN PLUS, use the DSTWU subroutine. In HYSYS.Plant, use **Short-cut Column.**

c. Using the design determined in a and b, simulate the towers; that is, solve the MESH equations. In ASPEN PLUS, use the RADFRAC subroutine. In HYSYS.Plant, use **Column.**

HYSYS.Plant Solution	ASPEN PLUS Solution

Exercise E.1 Reactor Design Problem

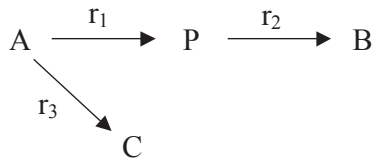
Maleic anhydride is manufactured by the oxidation of benzene over vanadium pentoxide catalyst (Westerlink and Westerterp, 1988), with excess air. The following reactions occur:

Reaction 1: $$C_6H_6 + \tfrac{9}{2}O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O \quad (1)$$

Reaction 2: $$C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O \quad (2)$$

Reaction 3: $$C_6H_6 + \tfrac{15}{2}O_2 \rightarrow 6CO_2 + 3H_2O \quad (3)$$

Since air is supplied in excess, the reaction kinetics are approximated as first-order rate laws:



$$r_1 = k_1 C_A, r_2 = k_2 C_P \text{ and } r_3 = k_3 C_A \quad (4)$$

In the above, A is benzene, P is maleic anhydride (the desired product), and B and C are the undesired byproducts (H_2O and CO_2), with kinetic rate coefficients in s^{-1}:

$$\left.\begin{aligned} k_1 &= 4{,}300 \exp\left[-25{,}000/RT\right] \\ k_2 &= 70{,}000 \exp\left[-30{,}000/RT\right] \\ k_3 &= 26 \exp\left[-21{,}000/RT\right] \end{aligned}\right\} \quad (5)$$

In Eq. (5), the activation energies are in kcal/kgmol.

The objective of this exercise is to design a plug flow reactor to maximize the yield of MA, for a feed steam of 200 kgmol/hr of air (21 mol % O_2 and 79 mol % N_2) and 2 kgmol/hr of benzene, at 200 ^oC and 1.5 Bar. Assume a reactor diameter of 2 m, neglect pressure drops, and design for adiabatic operation.

a) For fixed reactor tube length of 7 m, define the optimum reactor feed temperature to maximize MA yield (Hint: check values in the range 700-800 ^oC)

b) Investigate the effect of both reactor tube length, in the range 5-15 m, and feed temperature, in the range 700-800 ^oC, on the MA yield. Define the optimum combination of both of these variables.

HYSYS.Plant Solution	ASPEN PLUS Solution