

# Aspen Plus Training



الجامعة الألمانية الأردنية  
German Jordanian University

**Dr. Ziad Abuelrub**



# OUTLINE

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1. **Introduction**
2. Getting Started
3. Thermodynamic Models & Physical Properties
4. Pressure Changers
5. Heat Exchangers
6. Flowsheet Analysis
7. Reactors
8. Equilibrium Separation Column

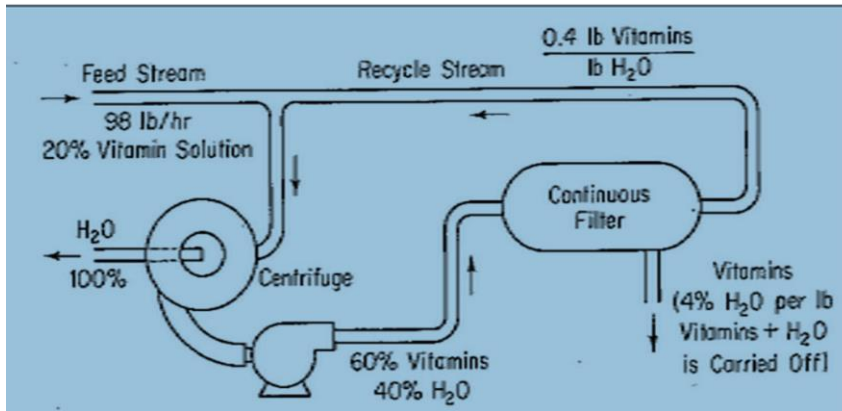
# ABOUT ASPENONE AND ASPENPLUS®



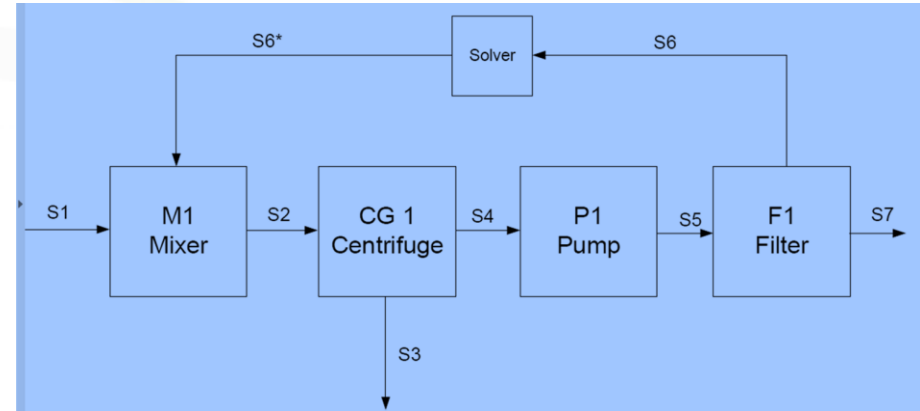
- AspenPlus® is a computer package (or software) provided by a US based company called AspenTech.
- The company develops several software packages that are sold under the name AspenONE which includes applications for engineering, supply chain, and manufacturing.
- This course will focus mainly on AspenPlus®, which we will refer from now on as Aspen, since it is the core element of AspenONE Engineering.
- This software provides many excellent features for process simulation. The following is some important features:
  - Best-in-class physical properties methods and data.
  - Improved conceptual design workflow.
  - Scalability for large and complex processes.
  - State of the art column internals calculations for flooding and pressure drop.
  - Rate-based distillation
  - Modeling batch distillation in a rigorous manner.
  - Polymer thermodynamics methods and data, rate-based polymerization reaction models, and a library of industrial process models.

- Computer programs are used to model chemical and other processes
- **CAD**: Computer Aided Design softwares
- Computers are only aiding in performing routine tasks that take time
- **Process Simulation**: the analysis of process flowsheets to determine the relations between the different items of that flowsheet.
- A process simulation software contains three main components:
  1. Material and energy balance equations
  2. Physical and thermodynamic properties of pure components and mixtures
  3. Model describing the unit operations
- Chemical Process simulators:
  - First appeared 1970s
  - Available in commercial and open source
  - Examples: AspenPlus®, Pro/II®, WinSim®, PromMax®, ...
  - Some softwares specialize in one process only (sulfur recover), while others (e.g. AspenPlus®) are more general applications

- There are two approaches in which simulation work:
  - **Sequential** (Most common): the simulator starts with the inlet streams, make sure it has zero degree of freedom (dof) and solve the first block. The results are used to solve the next block and so on.
  - **Equation based** (less common): the simulator writes all equations for all unit operations (given dof=0) and solve all equations simultaneously.
- The simulation flowsheet is based on **blocks** rather than unit operations
- Blocks vs. Unit Operations:
  1. Only units that have a model in the program are included. Some units are too complicated to be included (e.g. particulate filter)
  2. Only units used during steady-state operations are included. Units of start up and maintenance are not included.
  3. Points of mixing and splitting are represented as blocks, which are not real units but necessary for the simulation to perform the material and energy balance
  4. Additional or imaginary blocks may used in the simulation (e.g. a block for an initial guess).



Vitamin Concentration Process



Simulation flowsheet for the vitamin Concentration Process

- Each stream is given a name and number
- Unit operations are represented as blocks (CG1, P1, F1)
- Two additional blocks are added (M1, Solver)
- Process simulators don't have to represent every unit operation in the plant
- We can neglect some unit operations without affecting the accuracy of the model
- A simulation flowsheet is not acceptable as a process flowsheet (PFD)
- Every software will only solve the system you define
- It is your responsibility to know in advance the suitable operating conditions thermodynamic model.

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# OBJECTIVES

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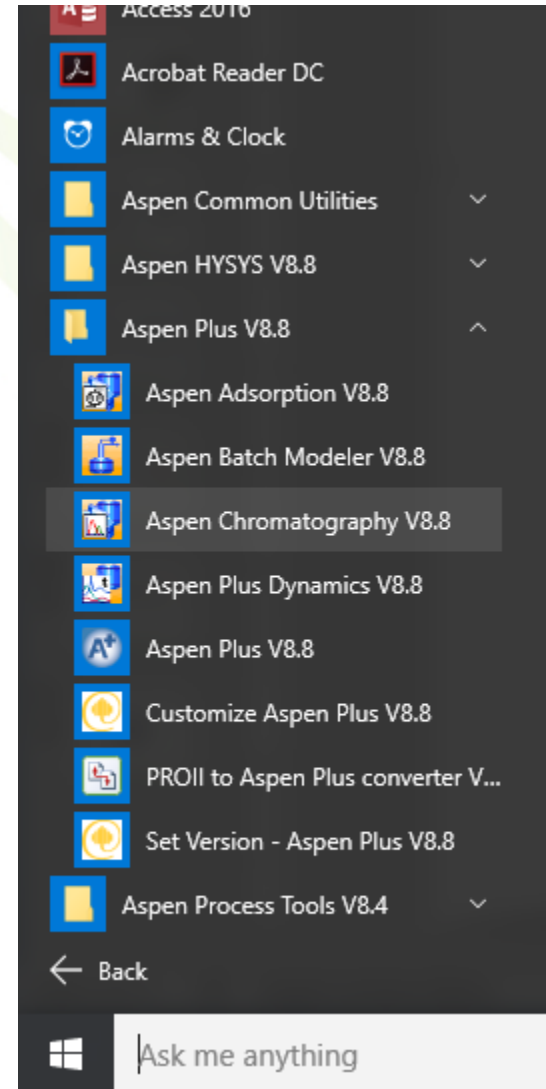


- Learn how to access Aspen Plus
- Introduce the Aspen Plus interface
- Learn how to draw flowsheets and input data
- Learn how to run a simulation and view results

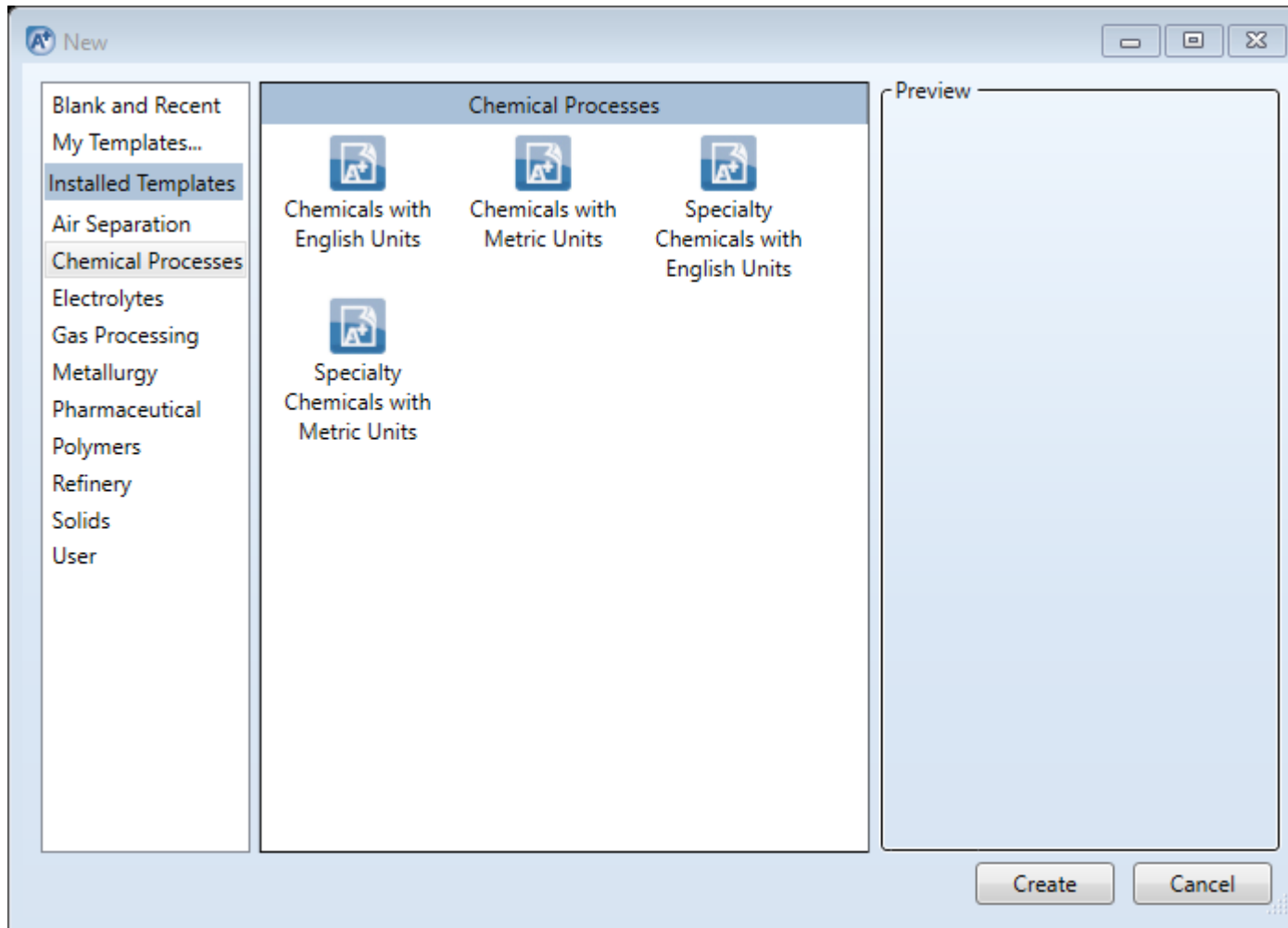
# ACCESSING ASPEN PLUS

from the **Start** Menu by going to **AspenPlus V8.8> AspenPlus V8.8**.

**Or add the icon to the :desktop**



# ACCESSING ASPEN PLUS



# ASPEN PLUS INTERFACE



The screenshot displays the Aspen Plus V8.8 software interface. The main window is titled "Simulation 1 - Aspen Plus V8.8 - aspenONE". The interface includes a menu bar (File, Home, View, Customize, Resources), a ribbon with various tool groups (Clipboard, Units, Setup, Components, Methods, Draw Structure, Tools, Data Source, Analysis, Run, Control Panel, Input, History, Report, Summary, Pure, Binary, Mixture, Ternary Diag, Residue Curves, PT Envelope, Analysis), and a Properties panel on the left. The Properties panel shows a tree view of the simulation components, with "Components" expanded to show "Specifications".

The "Components - Specifications" window is active, showing a table for selecting components. The table has the following columns:

| Component ID | Type | Component name | Alias |
|--------------|------|----------------|-------|
|              |      |                |       |

Below the table are buttons for "Find", "Elec Wizard", "User Defined", "Reorder", and "Review".

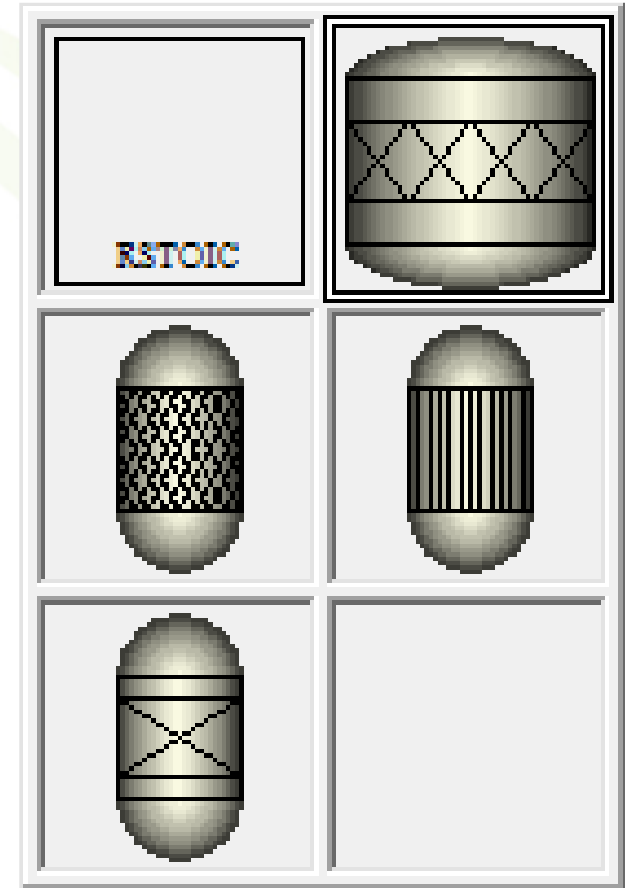
At the bottom of the interface, a status bar indicates "Required Input Incomplete" and a "Check Status" button. The zoom level is set to 100%.

The screenshot displays the AspenONE software interface in the Flowsheet tab. The top menu bar includes File, Home, Economics, Dynamics, Equation Oriented, View, Customize, Resources, Modify, and Format. The main workspace is currently empty, showing a 'Main Flowsheet' window. On the left, a 'Simulation' tree lists various project components like Setup, Property Sets, Analysis, Flowsheet, Streams, Blocks, Utilities, Reactions, Convergence, Flowsheeting Options, Model Analysis Tools, EO Configuration, Results Summary, and Dynamic Configuration. Below the simulation tree are sections for Properties, Simulation, Safety Analysis, and Energy Analysis. At the bottom, a 'Model Palette' contains icons for Material, Mixer, FSplit, and SSplit. A status bar at the bottom left indicates 'Flowsheet Not Complete' with a 'Check Status' button, and the bottom right shows a zoom level of 150%.

| Economics    |              | Energy                   |             | EDR Exchanger Feasibility |    |         |
|--------------|--------------|--------------------------|-------------|---------------------------|----|---------|
| Capital Cost | Utility Cost | Available Energy Savings |             | Unknown                   | OK | At Risk |
| USD          | USD/Year     | MW                       | % of Actual | 0                         | 0  | 0       |

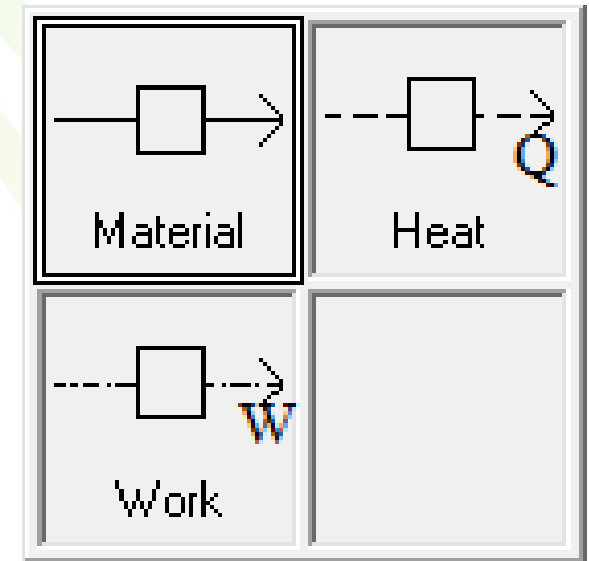
# 1. MODEL LIBRARY

- This is where the unit operations are presented
- Divided into tabs
- Under each tab, there are several models (icons) present a certain type of that unit operation.
- Example:
  - Reaction tab, Under which different models to calculate reaction products:
    - Rstoic
    - RYield
    - REquil
    - RGibbs
  - **RStoic** model has icons given in the picture for reorientation purposes.
  - You can switch between icons by Ctrl+K



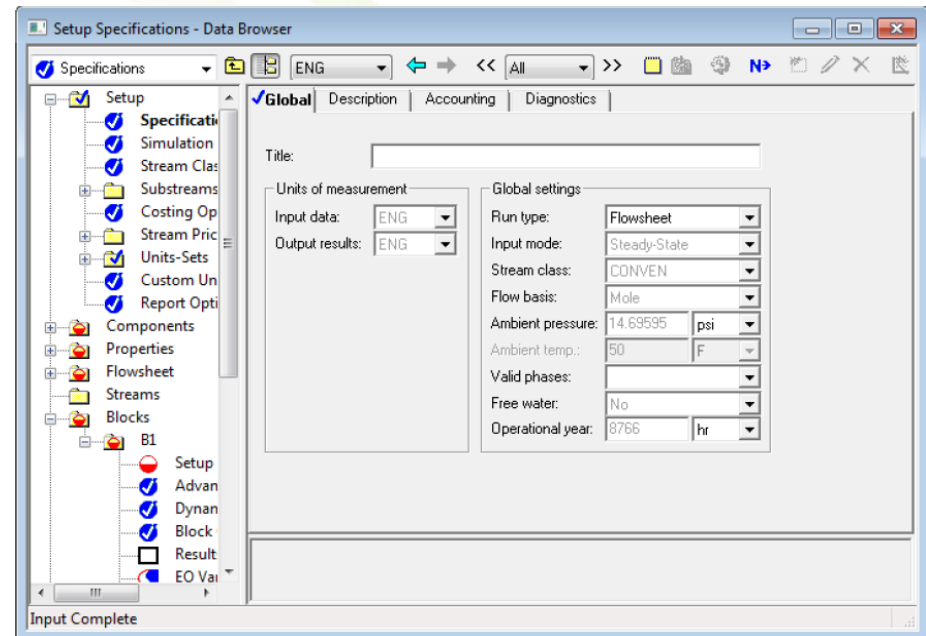
## 2. SELECT MODE BUTTON

- Once you place a model on the flowsheet, you can adjust the model's icon position, resize it, or delete it, or you can draw process stream connections.
- If you want to do any adjustments to the icon, you need to make sure the Select Mode button is clicked.
- If you want to connect process streams to the model, you need to click the STREAMS button (located below the Select Mode button).
- By default, clicking the STREAMS button will activate the Material stream, which is similar to a process stream in process flowsheet.
- Material streams contain all the information about what is being transferred in that stream in terms of composition, flow rate, and other thermodynamic and physical properties.
- Other types of streams in Aspen Plus (and simulation software in general) are the energy and work stream.



### 3. DATA BROWSER TOOLBAR

- The icons on this toolbar will open different pages of a window called Data Browser.
- The Data browser is where all the process information is input from the thermodynamic model used, the components, physical properties, streams information, units' information, and others.
- The data browser is divided into folders, under each folder there are several sheets, and in each page there are several tabs. Within these tabs you can control all features of your simulation.



Data Browser



## 4. SIMULATION RUN TOOLBAR

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- Contains buttons that will allow you to run, pause, stop, and debug your simulation once you have completed the flowsheet creation.
- have different buttons activated/deactivated depending on the status of the flowsheet.

## 5. FLOWSHEET STATUS BAR

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- This is located at the lower right corner of the window and indicates the status of the flowsheet.
- When you start a flowsheet, the message shown will be “**Flowsheet Not Complete**”, indicating that there are missing streams that need to be connected.
- Once you make all necessary connections, the message will change to “**Required Input Not Complete**”, indicating that you have not specified all required inputs.
- There are several messages that will appear as you work with your simulation, but, in general, your ultimate goal is to get the “Results Present” message, indicating that the simulation was performed successfully.

# HELP

- Remember always to use the help provided with Aspen Plus when you are in doubt or when you are not sure how to perform certain tasks.
- The help can be accessed from the Help menu or via the Help button ( ).



# OUTLINE

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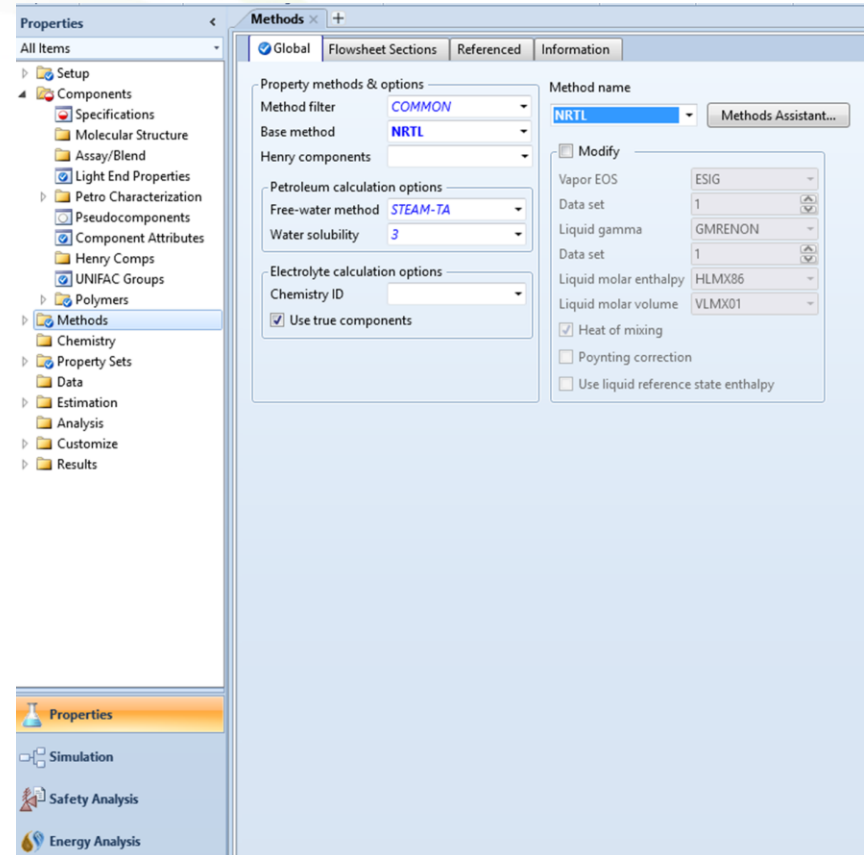


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- Selecting the proper method for estimating properties is one of the most important steps that will affect the simulation.
- The estimation methods are stored in what is called a “Property Method”
- A property method is a collection of estimation methods to calculate several
  - **thermodynamic properties:** fugacity, enthalpy, entropy, Gibbs free energy, and volume
  - **Transport properties** : viscosity, thermal conductivity, diffusion coefficient, and surface tension

# PROPERTY METHOD SELECTION

- Property methods can be selected from the Data Browser, under the Properties folder
- Peng-Robinson, Soave-Redlich-Kwong, and Perturbed Chain methods are the most commonly used methods with hydrocarbon systems such as those involved in the oil and gas industries.
- When you select a property method, you are in effect selecting a number of estimation equations for the different properties.



The screenshot shows the 'Methods' configuration window in a software application. The left sidebar displays a tree view under 'Properties' with folders for 'Setup', 'Components', 'Specifications', 'Molecular Structure', 'Assay/Blend', 'Light End Properties', 'Petro Characterization', 'Pseudocomponents', 'Component Attributes', 'Henry Comps', 'UNIFAC Groups', 'Polymers', 'Methods', 'Chemistry', 'Property Sets', 'Data', 'Estimation', 'Analysis', 'Customize', and 'Results'. The 'Methods' folder is selected.

The main window has tabs for 'Global', 'Flowsheet Sections', 'Referenced', and 'Information'. The 'Global' tab is active. The 'Property methods & options' section includes:

- Method filter: COMMON
- Base method: NRTL
- Henry components: (empty)
- Petroleum calculation options:
  - Free-water method: STEAM-TA
  - Water solubility: 3
- Electrolyte calculation options:
  - Chemistry ID: (empty)
  - Use true components

The 'Method name' section shows 'NRTL' selected in a dropdown menu, with a 'Methods Assistant...' button next to it. Below this is a 'Modify' section with several options:

- Modify
- Vapor EOS: ESIG
- Data set: 1
- Liquid gamma: GMRENON
- Data set: 1
- Liquid molar enthalpy: HLMX86
- Liquid molar volume: VLMX01
- Heat of mixing
- Poynting correction
- Use liquid reference state enthalpy

At the bottom of the interface, there is a navigation bar with icons for 'Properties', 'Simulation', 'Safety Analysis', and 'Energy Analysis'.

# PENG-ROBINSON EQUATION

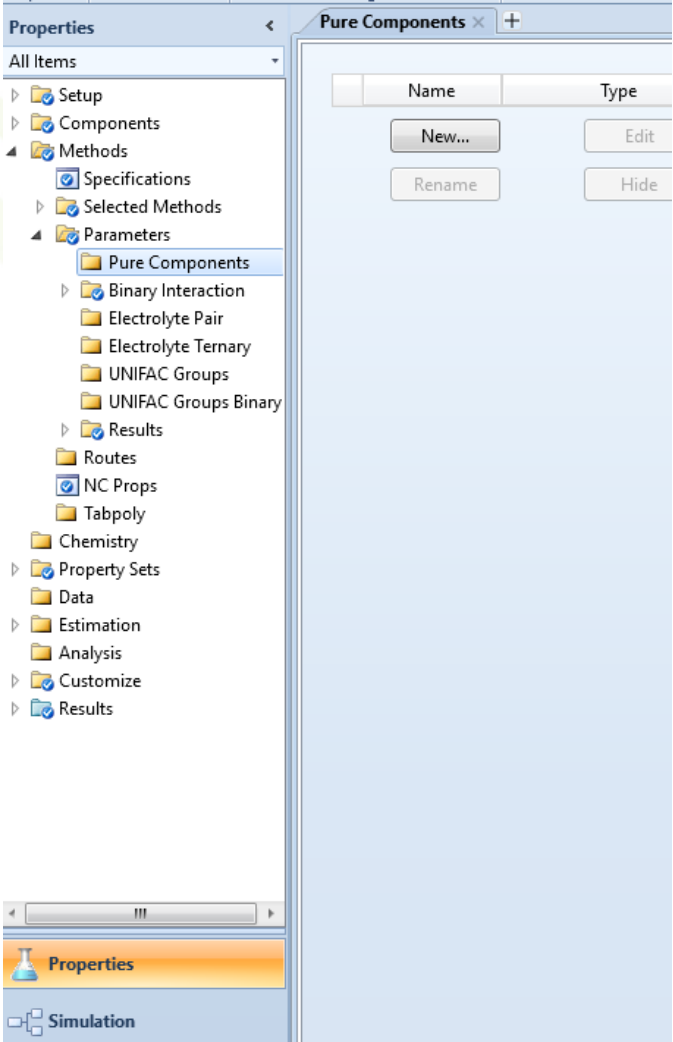
- For example, when you select the Peng-Robinson equation, you can see that the equation of state (EOS) selection is set to PENG-ROB which is given by:

$$P = \frac{RT}{(c + V_m) - b} - \frac{a}{(V_m + c)(V_m + c + b) + b(V_m + c - b)}$$

- Where  $a$ ,  $b$ , and  $c$  are component specific parameters.
- The values of these parameters are stored in Aspen Plus database for pure components or calculated using mixing rules for mixtures.

# DETERMINING HOW PROPERTIES ARE ESTIMATED

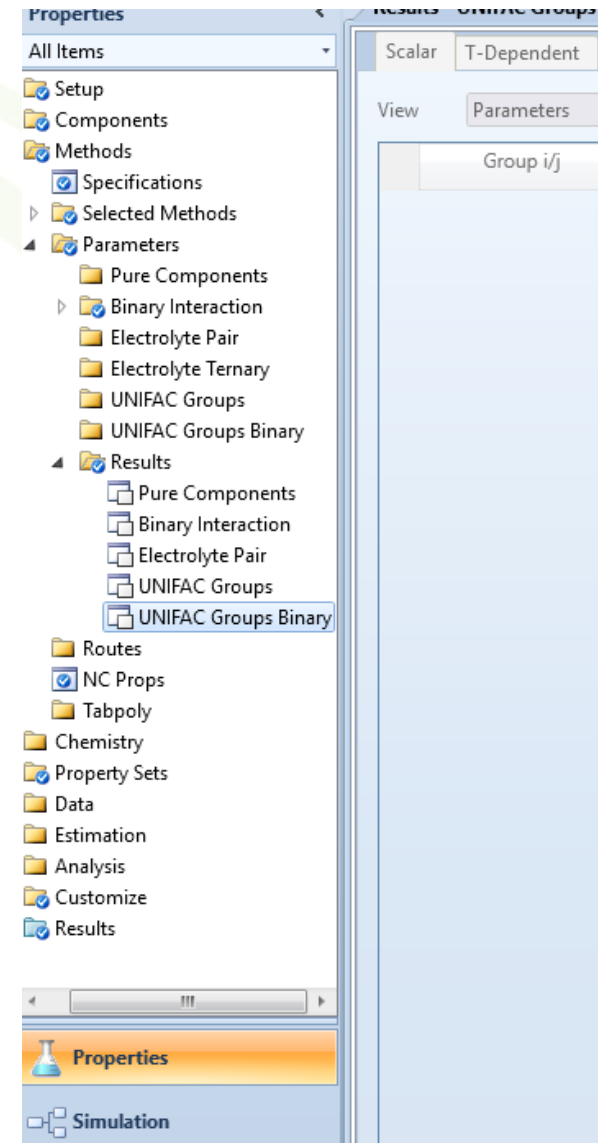
- When you select a component to be included in the simulation, many properties for this component will be loaded.
- A large number of the properties are loaded under the Parameters subfolder in the Properties folder.
- If you expand the Parameters subfolder, you will see that it consists of subfolders for Pure Component (where properties for the component itself, like heat capacity, heat of formation, etc are stored as shown in the snapshot to the right), Binary Interaction (where interaction parameters of the component with other loaded components are stored for different calculations), Electrolyte Pair (for electrolytic interaction parameters), and so on.
- Let us examine the Pure Component folder. As you can see in the snapshot above, the properties are denoted by a short name. For example, CPIGDP property is a short





# VIEW COMPONENT PROPERTIES

- If you are interested in view all properties of pure components, you can use Aspen Plus “Retrieve Parameter Results...” from the Tools menu.
- This option allows you to extract all properties of pure components used by Aspen Plus, even the ones not displayed by default.
- Once you activate the Retrieve Parameter Results option, you can navigate in the Data Browser to the Properties>Parameters>Results folder, where the results for pure components, binary interaction parameters,



# PHASE EQUILIBRIUM CALCULATIONS

- One of the key calculations performed in process simulations
- The basic principle of several unit operations (such as flash tanks, distillation columns, extraction...) is based on multi-phase equilibrium.
- Phase equilibrium is calculated using the **fugacity** (a measure of the tendency of a component to leave its phase).
- Equilibrium is achieved when the fugacity of the component is equal in all phases.

$i$  in liquid phase is given by:

$$f_i^L = \phi_{i,L} x_i P$$

and in the vapor phase:

$$f_i^V = \phi_{i,V} y_i P$$

where  $\phi_i$  is the fugacity coefficient.

At equilibrium  $f_i^L = f_i^V$ .

For pure components  
 $\phi_i^o P$ , since  $x_i$  and  $y_i$  are both 1.

# FOUR SYSTEMS OF CALCULATING FUGACITIES

## 1- IDEAL MODEL



- An ideal system is a system composed of ideal gases and liquids.
- An ideal gas follows the ideal gas law ( $PV = NRT$ ) and has a fugacity of 1.
- An ideal liquid has an activity coefficient ( $\gamma$ ) of 1.
- Ideal behavior can be assumed for vacuum/low pressure or very high temperature operations, for gases, and when very small interactions (or interactions that cancel each other) in liquids.
- In Aspen Plus, ideal behavior is modeled using the IDEAL property method.
- This method sets the activity coefficient for the liquid phase to 1, the EOS to the ideal gas law, and estimates the molar volume of liquids using the Rackett model.
- You can also use Henry's law with the ideal model by designating relevant components as Henry's components.
- **As a general rule of thumb, when you have systems involving material such as water, organic acids, amines, alcohols, esters, ketones, aldehydes, and/or ethers, then you are dealing with polar molecules and there is a very good chance that the system deviates considerably from ideality. Think, for example, of water/alcohol mixtures.**

# FOUR SYSTEMS OF CALCULATING FUGACITIES

## 2- EQUATION OF STATE MODELS



- an equation of state (EOS) is a PVT relation used to predict thermodynamic properties.
- In Aspen Plus, there are several equations of state used for different applications, examples:
- the Peng-Robinson EOS (and its variations)
- the Soave-Redlich-Kwong EOS (and its variations), which belong to the cubic EOS.
- Other forms of EOS include those derived from statistical thermodynamics such as the Sanchez-Lacombe and SAFT.
- Another form of the EOS models is the steam tables (provided as a Base model in Aspen Plus).

- For non-ideal liquid solutions, the fugacity of the components in the solution deviates from that of the pure component.
- The ratio of the fugacity in solution to that of pure component is defined as the activity:

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

- The activity can be calculated from the activity coefficient ( $\gamma$ ) as follows:

$$a_i = \gamma_{i,L} \cdot x_i$$

- In general, the activity coefficient is greater than unity. What this means is that the fugacity of a component in mixture is higher than that of pure component. Thus, the same liquid will have higher tendency to vaporize when in mixture than in its pure state. This can be attributed to the increased repulsion between molecules with mixtures. In few cases, the activity coefficient will be less than unity, indicating increased attraction between molecules and less tendency to vaporize.
- In Aspen Plus, there are several activity coefficient models. Among the most commonly used is the
- NRTL, which can be applied to polar mixtures.
- Other models include: Wilson, Van Laar, UNIFAC, UNIQUAC, Flory Huggins, Electrolyte NRTL, and Scatchard Hildebrand models. In these models, the activity coefficient approach is used to calculate the liquid properties, while the vapor phase properties are calculated using an equation of state.

- There are still many other property models available through Aspen Plus.
- These models are classified as “Vapor Pressure and Liquid Fugacity Models” and have found applications in specific processes.
- Among these models are:
  - API sour model (developed for sour water treatment applications),
  - Chao-Seader and Grayson-Streed models (applicable to heavy hydrocarbon systems),
  - Kent-Eisenberg model (for amine sweetening units).

# MODEL SELECTION

- In general, different industries tend to accumulate experience on which model best fits its system.
- For example, from experience we now that the PR and the SRK models fit the oil and gas processing systems very well.
- You can always check the Help files for more recommendations about the use of property packages.
- As a general guideline you can refer to the chart in Figure 15.
- The main criterion here is the present of polar compounds (water, alcohol, acids...). If this is the case, then non-ideality is expected and we refer to the activity coefficient models. Also, be aware of any non-condensable components (CO<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>...) which require special treatment using Henry's law.

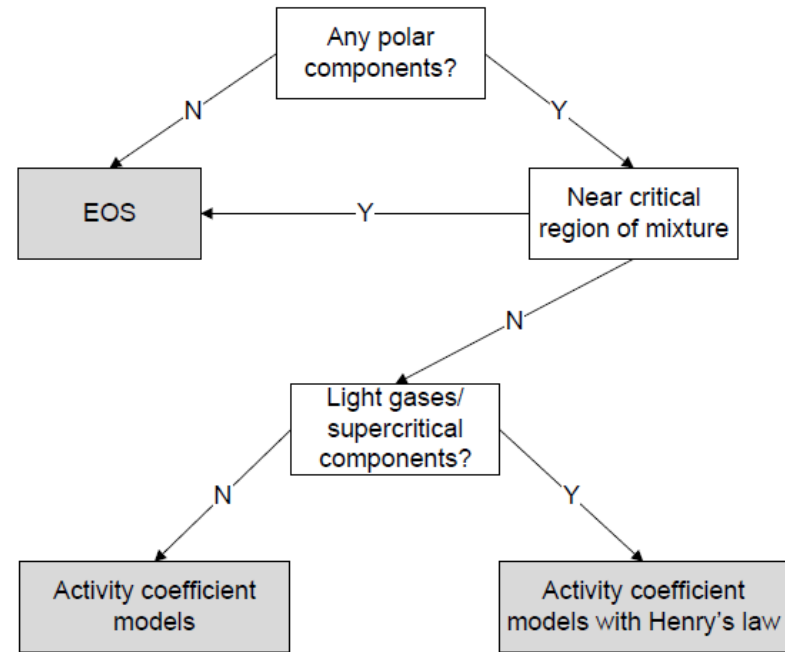


Figure 15. Selecting a property method.

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# PRESSURE CHANGERS

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- The modules in this library deal with parts of the process that has an effect on changing the pressure either directly, such as pumps or compressors, or through its operation, such as pipes and pipelines.
- It is usually required when handling fluid streams to change its pressure for different reasons. For example, in the gas sweetening plants, an absorption column might be needed to operate at high pressures to improve the absorption and a pump might be used to compress the inlet fluids to the desired value. On the other hand, the regeneration column must be operated at near atmospheric conditions to allow the adsorbed gases to leave the liquid. The liquid which comes from the absorption column at high pressures is passed through a valve to achieve the design pressure.
- Other operations require transportation of fluids. During transportation, hydrostatic pressures and friction causes a pressure drop. Therefore, pumps and compressors are needed to provide the required energy, by increasing the pressure, to the required level. The friction losses in pipes are a common cause for pressure drop, especially when with long pipelines. Therefore, pressures drops must be calculated to determine the required pumping through the pipelines, which is a common calculation when dealing with pipe networks (specifically for oil and gas collecting systems).

- In general, a pump is a device used to transport liquids, gases, and slurries. However, the term pump is usually used to refer to liquid handling equipment (this is true with Aspen Plus). The purpose of the pump is to provide a certain pressure at certain flow rate of a process stream. The pressure requirement is dictated by the process and piping involved, while the flow rate is controlled by the required capacity in the downstream units.
- There are several types of pumps used for liquid handling. However, these can be divided into two general forms: positive displacement pumps (including reciprocating piston pump and the rotary gear pump), and centrifugal pumps. The selection of the pump type depends on many factor including the flow rate, the pressure, the nature of the liquid, power supply, and operating type (continuous or intermittent). Figure 30 shows a general guideline to selecting pump type based on flow rates and discharge pressure. Centrifugal pumps, such as the one shown in Figure 31, are by far the most widely used type in the chemical process industry, with other types employed for special process specifications (e.g., high pressures).

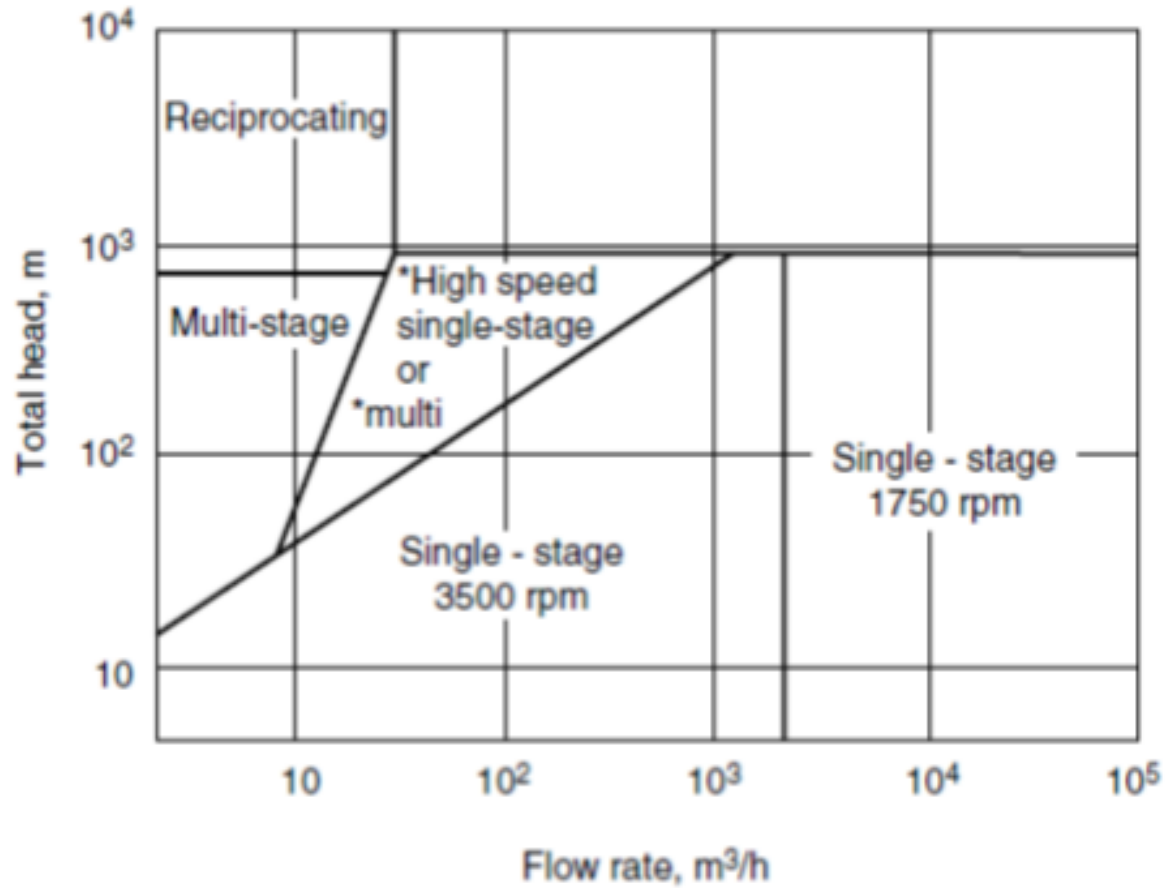
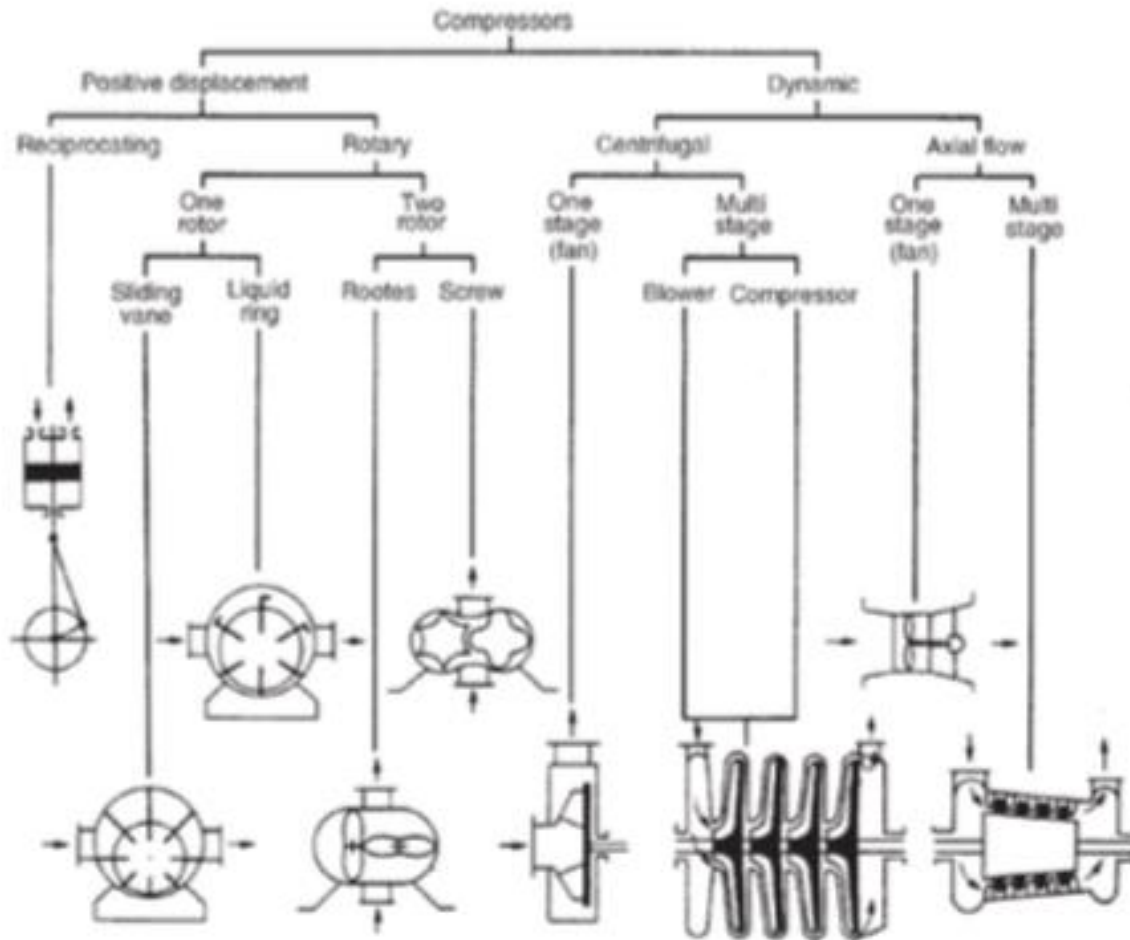


Figure 30. Pump selection guide. <sup>2</sup>

# COMPRESSORS



- The principles of gas compression are similar to that of liquid pumping. The main difference lies in the mechanical design of the equipment due to the differences in the physical properties between gases and liquids. Common compressor types are shown in Figure 35. Since gases are much more compressible than liquids, the compression process gives rise to higher temperature and volume changes in the gas.



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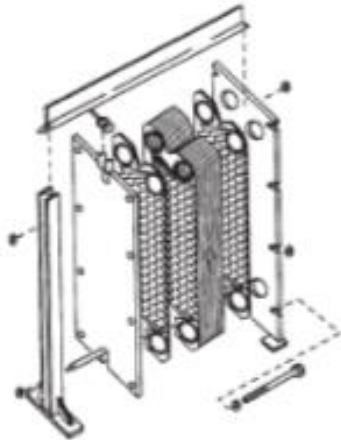
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# HEAT EXCHANGERS

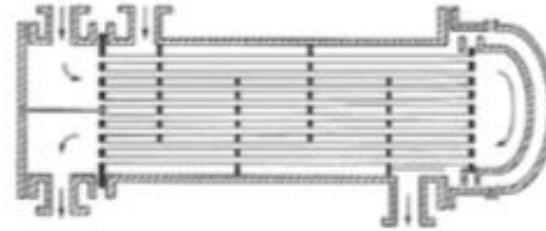
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There are many types of heat exchangers applied in the process industry. These types include:

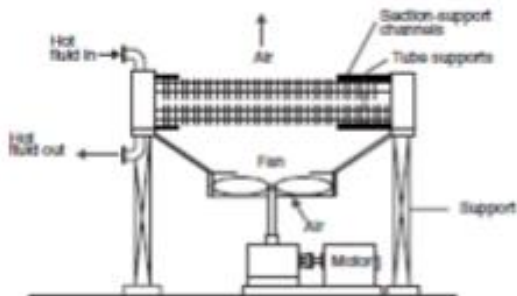
- Hairpin/Double pipe exchangers
- Shell and tube exchangers
- Plate and frame exchangers
- Plate-fin exchangers
- Spiral heat exchangers
- Air coolers and condensers
- Direct contact (quenching towers)
- Fired heaters



(a) Plate and frame exchanger<sup>8</sup>



(b) Shell and tube exchanger<sup>9</sup>



(c) Air coolers<sup>10</sup>



(d) Double pipe exchanger<sup>11</sup>

(12)

$$Q = m\Delta H_{hot} \cong mC_p(T_{in}^{cold} - T_{out}^{cold})$$

Figure 42. Different types of heat exchangers



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- One of the most useful functions of process simulators is the ability to manipulate and analyze the different design variables to determine the required value or study its effect on the process. In addition, calculations of certain values, such as conversion and yield, might sometimes be necessary although the results are not included in the simulation output. Another feature that is usually necessary is to optimize a process based on certain criteria.
- The above features are available in Aspen Plus under the Flowsheeting Options and Model Analysis Tools. The following sections will discuss some of these features.
- Analysis tools:
  - Sensitivity analysis
  - optimization

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- Reactions are usually the heart of the chemical processes in which relatively cheap raw materials are converted to more economically favorable products. In other cases, reactions play essential safety and environmental protection roles. In any case, proper design and operation of the reactor is required to provide the desired outcome. Such design is usually based on thermodynamics, chemical kinetics, and transport studies coupled with experience and economic considerations.
- When studying chemical reactions we need to determine what are the reactants and products needed, to what extent will the reaction proceed, and how fast it will proceed. The study of such factors in addition to the detailed design of the reactor consist the chemical reaction engineering field in which process simulation can be of great help.
- Aspen Plus provides several libraries to model reactive processes. The selection of the model depends on the amount of information available and the type of simulation.

# MATERIAL BALANCE ON REACTIVE PROCESSES

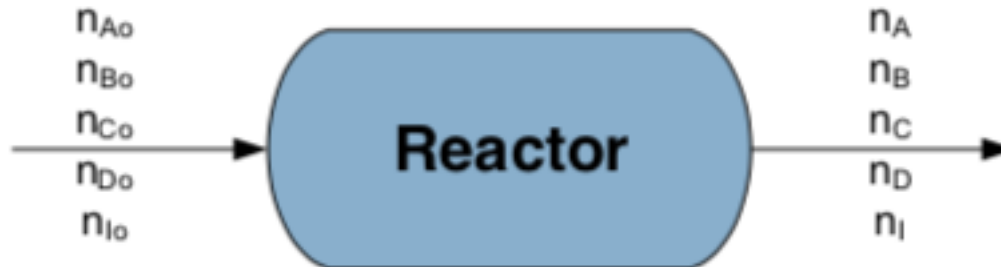
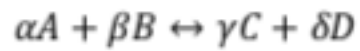


Figure 67. Simple reactor block.

# REACTOR MODELING IN ASPEN PLUS

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There are seven blocks for reaction modeling in Aspen that can perform calculations based on:

- RStoic: stoichiometry
- Ryield: yield
- Requil: equilibrium
- Rgibbs: minimum Gibbs free energy
- RCSTR and RPlug: kinetics models for CSTR and PFR
- batch model is available for batch reactors

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# EQUILIBRIUM SEPARATION COLUMN

In equilibrium separation processes, two or more coexisting zones are created with preferential distribution of the different components involved in the process in each zone. For example, in distillation a liquid and vapor zones are created and the components are separated in different proportions between these zones. In absorption and stripping, liquid and gas phases are created. In extraction, two liquid phases are created. The zones are assumed to be, as the name implies, in equilibrium with each other. This means that the temperature, pressure, and phase compositions are all in thermodynamic equilibrium. Thus, while all separation processes are essentially a mass transfer process, the equilibrium assumption cancels out the need for dealing with transfer rates and focuses only on the transfer amounts.

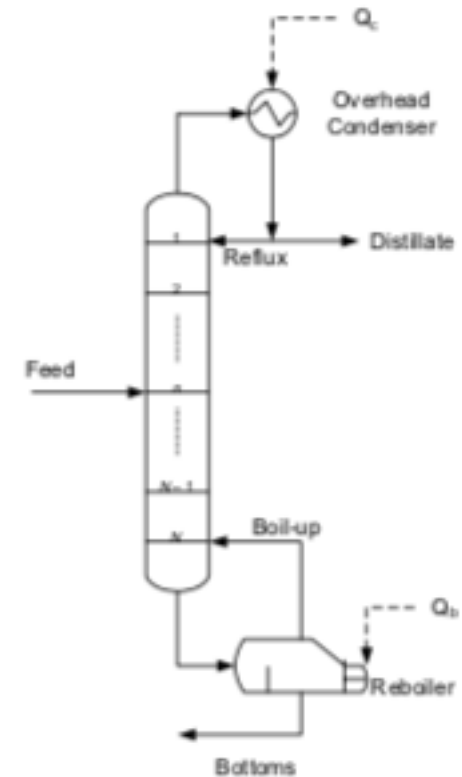


Figure 74. Simple, continuous distillation column



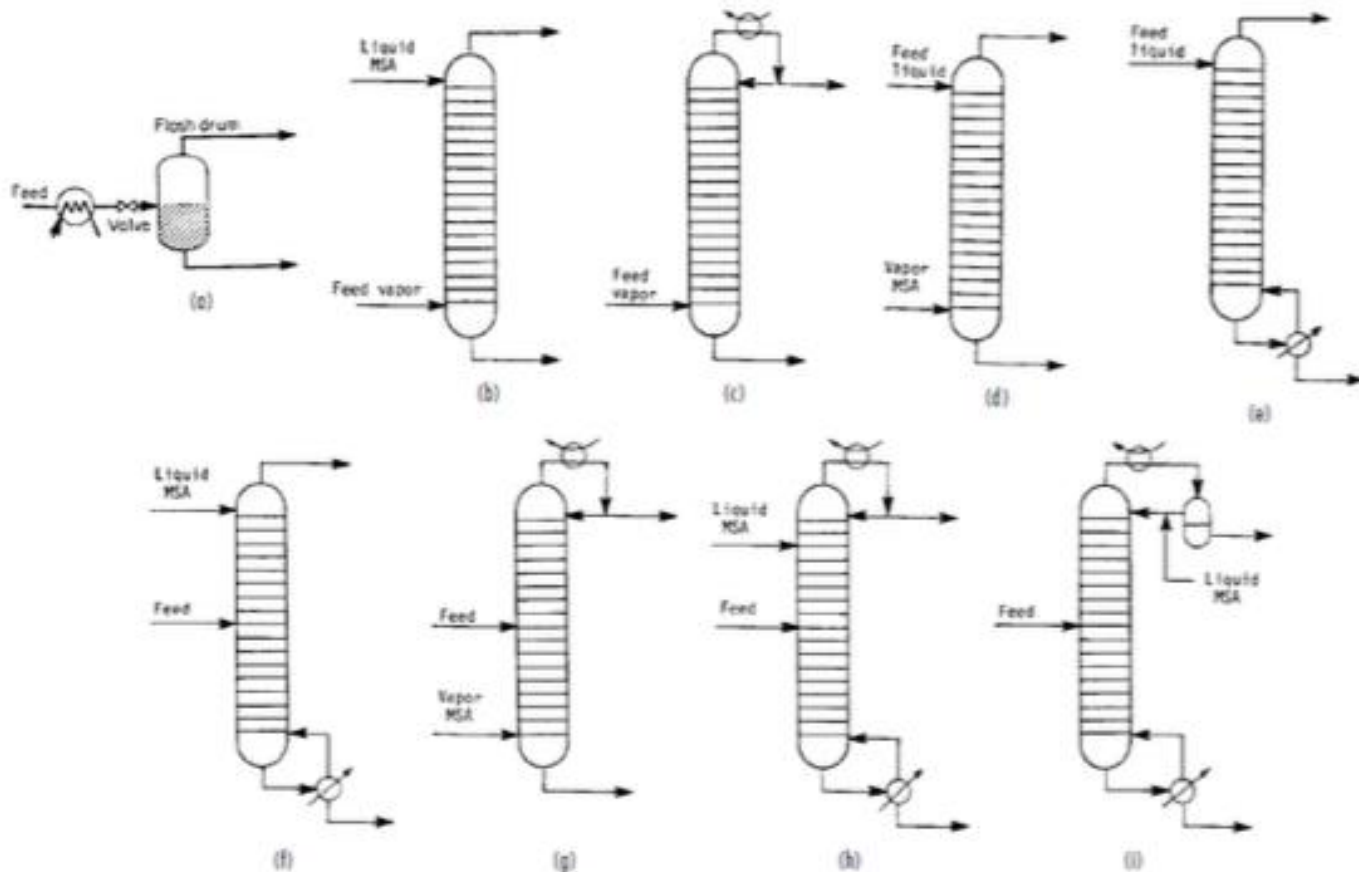


Figure 75. Separation operations related to distillation. (a) Flash vaporization or partial condensation. (b) Absorption. (c) Rectifier. (d) Stripping. (e) Reboiled stripping. (f) Reboiled absorption. (g) Refluxed stripping. (h) Extractive distillation. (i) Azeotropic distillation.<sup>20</sup>

# SEPARATION COLUMN IN ASPEN PLUS

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Aspen Plus provides several modules for multistage separation processes. These models are the :

- DSTWU
- Distl
- RadFrac (which are shortcut and rigorous methods for distillation, absorption, and stripping application)
- Extract (for extraction applications)
- MultiFrac
- SCFrac
- PetroFrac (for advance fractionation applications)
- BatchSep (for batch distillation).

# REFERENCES

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- Aspen plus help
- Aspen Plus® Lab Manual
- Handout exercises