Project Report on

PROCESS SIMULATION & MODELING IN ASPEN PLUS

By

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DECLARATION BY THE CANDIDATE

I, **SAYAN DEORI**, the undersigned solemnly declare that the project report titled

PROCESS SIMULATION & MODELING IN ASPEN PLUS

is based on my own work carried out during the course of our study under the supervision of **Mr. NISHESH JYOTI RAO**. I assert the statements made and conclusions drawn are an outcome of my own work. I further certify that:

The work contained in the report is original and has been done by me under the general supervision of my supervisor.

The work has not been submitted to any other Institution for any other degree/diploma/certificate in any University of India or abroad.

We have followed the guidelines provided by the university in writing the report.

SAYAN DEORI

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ACKNOWLEDGMENT

I would like to thank, Mr. Nishesh Jyoti Rao for helping and motivating me throughout the process of my project. I would also like to specially thank the Chemineers team for this wonderful opportunity. I would also like to thank Shubh Maheshwari for being a wonderful guide during the course of this project. And, lately, I would like to thank my fellow batchmates who helped me by sharing ideas together. It would not have been possible without them.

SAYAN DEORI

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OBJECTIVE

To get a basic exposure in Aspen Plus. It'll help us to predict flowrates, compositions and physical properties of the process streams, operating conditions of process, sizing of equipment & producing economical and quality products while process designing of an Industrial plant.

INTRODUCTION

Process Simulation is the Art of Modelling Chemical and Physical Processes in Computer. Process simulation is used for the design, development, analysis, and optimization of technical processes such as: chemical plants, chemical processes, complex manufacturing operations and similar technical functions.

Process simulation is a **model**-based representation of chemical, physical, biological, and other technical processes and unit operations in software. Basic prerequisites for the model are chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models which, in combination, allow the calculation of process properties by the software.

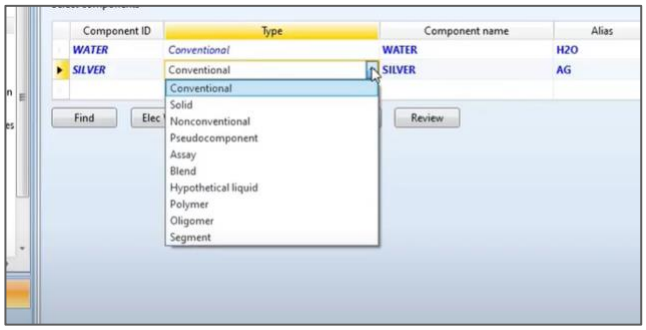
Process simulation software describes processes in flow diagrams where unit operations are positioned and connected by product streams. The software solves the mass and energy balance to find a stable operating point on specified parameters. The goal of a process simulation is to find optimal conditions for a process. This is essentially an optimization problem which has to be solved in an iterative process.

Model development is done through the principles of chemical engineering but also control engineering and for the improvement of mathematical simulation techniques. Efforts are made to develop new and improved models for the calculation of properties.

There is a famous process modelling tool, **Aspen Plus** which is used for process monitoring, optimization and conceptual designing, specially by chemical process industries. With over 1550 pure components, 1000 VLE, 3000 LLE binary database and 60 models of thermodynamic methods, it is considered as a designer's delight that helps in designing the plant in an easy user-friendly way.

COMPONENT TYPES

There are various component types in Aspen Plus which helps the user analyse and simulate systems. A few of the components are conventional, solid, non – conventional, pseudocomponent, assay, blend, polymers, oligomer and segment, and hypothetical liquid.



Conventional: Typical components that may participate in vapour-liquid phase equilibrium.

Solid: Single species solids whose properties are calculated by solid-based models.

Non-conventional: Solids that are not pure chemical species.

Pseudocomponent, Assay, Blend: Components representing petroleum fractions, characterised by boiling point, molecular weight and other properties.

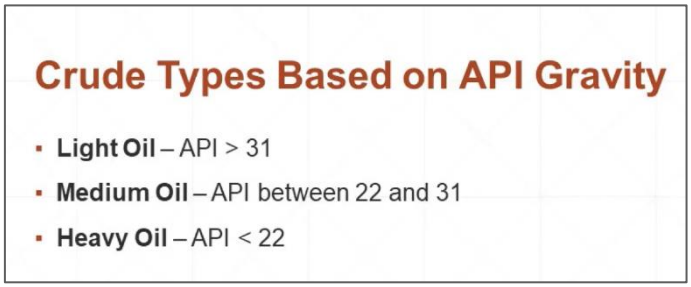
Polymers, Oligomer, and Segment: Components used in polymer models.

Hypothetical liquid: A component type that is mainly used in pyrometallurgical applications when modelling a component as liquid.

API GRAVITY – AMERICAN PETROLEUM INSTITUTE

It is used to demonstrate how density of crude oil compares to density of water.

$$API\ Gravity = \frac{141.5}{SG} - 131.5$$



Higher API **indicates a lighter (lower density) crude**. Lower API indicates a heavier (denser) crude. Generally, lighter (high API) crudes are more valuable because they yield more high-value light products when run through a refinery.

AVAILABLE PROPERTIES TABLE

Let us discuss about the available properties that will help us in simulations while using Aspen Plus. The table mostly contains properties, units, feed and products.

Available properties

PROPERTIES	UNIT	FEED	PRODUCTS			
		F-VGO	L-NAPH	H-NAPH	P-DZL	P-VGO
Sulfur	ppm wt	2	<5	<20	<20	<200
Density	Kg/m3	929.3	742	801	835	845
Distillation vol%		D1160	D86	D86	D86	D1160
IBP	°C	364	65.72	163.72	242.2	369.84
D10	°C	397	85.29	170.17	250.57	385.05
D30	°C	428	101.04	174.65	267.93	411.89
D50	°C	460	114.25	178.76	290.02	438.35
D70	°C	500	124.26	182.89	316	473.54
D90	°C	548	131.12	187.31	342.07	529.7
D95	°C	555	132.66	190.63	347.51	555.61
FBP	°C	594	134.21	193.95	352.95	581.62

R.C Patil et al. / Computers and Chemical Engineering 104 (2017) 89-106.

| Figure |

To model and simulate a flow system such that the product that we get out of the model will have the same properties as the desired one, we need the knowledge of Available Properties.

In the feed column, we can see F-VGO which is Vacuum Gas Oil. It is the bottom product of vacuum distillation column. This is not a valuable product. So, to make it valuable, it has to be cracked and broken into smaller chain hydrocarbon so that we can get valuable products. So, it has to be sent to *FCC* or hydro catalytic reactor. Products are L-NAPH, H-NAPH, R-DZL (Diesel) and P-VGO.

Crude oil also contains many impurities and the most poisonous among them is sulphur since it deactivates the catalyst. The data is given in the table for sulphur in ppm wt. Distillation volume percentage gives us the percentage of feed that has gone through distillation.

IBP or Initial Boiling Point gives us the boiling point of the distillate. D10 means its 10% volume has been separated as the distillate. It means the lighter components have been separated in the form of distillate. As we go down the table, we come across D90 which contains compound with higher initial boiling point. This is because, as we move down, we get compounds with higher hydrocarbons which has higher initial boiling point.

FBP or Final Boiling Point is the stage when 100% of the feed distillates. L-NAPH, H-NAPH, R-DZL AND P-VGO are good grade products.

PROPERTY METHODS

Property methods are a collection of models and methods used for calculating the physical properties of components via thermodynamic and transport properties.

Transport Properties	Thermodynamic Properties
• Mass (diffusion coefficients) • Heat (thermal conductivity, convective heat transfer coefficients) • Momentum (surface tension, viscosity)	• Physical (density, molecular weight, enthalpy, entropy, Gibbs free energy) • Phase equilibrium (fugacity coefficient, chemical potential)

| Table |

Transport Properties: Although we touched on some of the options for including selected physical properties in stream tables, we did not touch on adding those properties that are important for mass transfer (i.e. diffusivities). However, diffusivity is not one of the default variables that are reported by Aspen and it is only reported if the user defines a specific property set. The easiest way to do this is to modify an existing property set that reports other parameters of interest and then have Aspen report this property set. Transport properties in Aspen Plus are mass (diffusion coefficient), heat (thermal conductivity, convective heat transfer coefficient) and momentum (surface tension, viscosity).

Thermodynamic Properties: Thermodynamic phase equilibrium can be determined in a number of ways, including chemical potential, fugacity, activities, activity coefficients, or the equilibrium distribution ratio. You will notice that the Ideal methods rely on using ideal system equations to calculate the equilibrium distribution ratio (K), which is then used to determine the equilibrium conditions.

Equation of State Property Methods. These methods use the various equations of state that are learned about in chemical engineering thermodynamics, to calculate the equilibrium distribution ratio. The two most familiar methods from this section are listed in the table below. You will also notice that Aspen provides many of the minor variations to the most common methods (i.e. PRMHV2 – a modified Peng-Robinson equation).

EOS Property Method	K – Value Method
• PENG-ROB • RK-SOAVE	• Peng-Robinson • Redlich-Kwong-Soave

| Table |

The next group of available property methods is the Activity Coefficient group. This group uses various relationships to calculate the liquid phase activity coefficient and then calculate the vapor fugacity using a second relationship.

Property Method	Liquid Phase Activity Coefficient	Vapor Phase Fugacity
• NRTL (Non-Random Two Liquid) • UNIFAC • VANLAAR • WILSON	• NRTL • UNIFAC • Van Laar • Wislon	• Ideal Gas • Redlish-Kwong • Ideal Gas

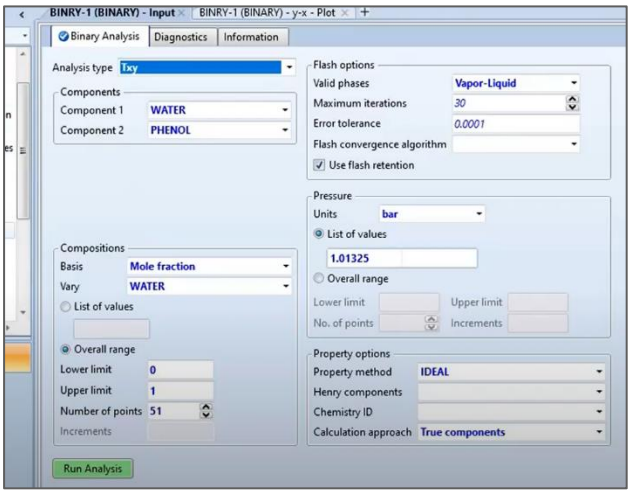
| Table |

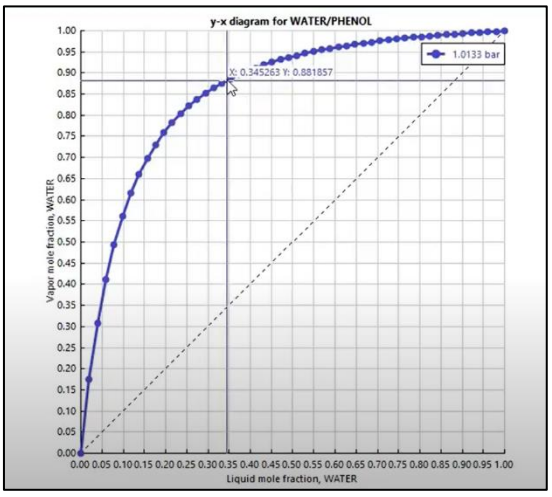
This is the Special Systems group. You will notice that this group provides the available methods for amine systems, solids systems, and steam systems.

Let us now do some practical work applying those previously mentioned property methods and see what we obtain as results.

WATER PHENOL SYSTEM IN IDEAL PROPERTIES

In Aspen Plus, select Binary Analysis. Now select component 1 as water and component 2 as phenol. The compositions with lower limit and upper limit will get filled



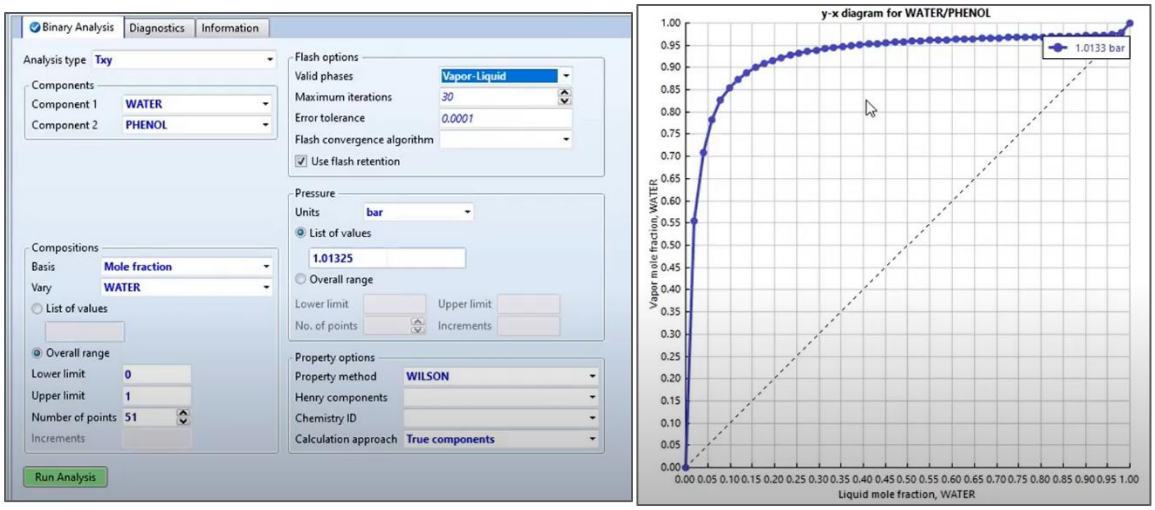


automatically. In the flash options box, select Vapor-Liquid for valid phases with maximum iterations 30. Now, In the property options box, under property method, select the method which needs to be applied, i.e. IDEAL (for this case). And then click on run analysis to obtain the required results and graph.

| Figure |

WATER PHENOL SYSTEM IN WILSON PROPERTIES

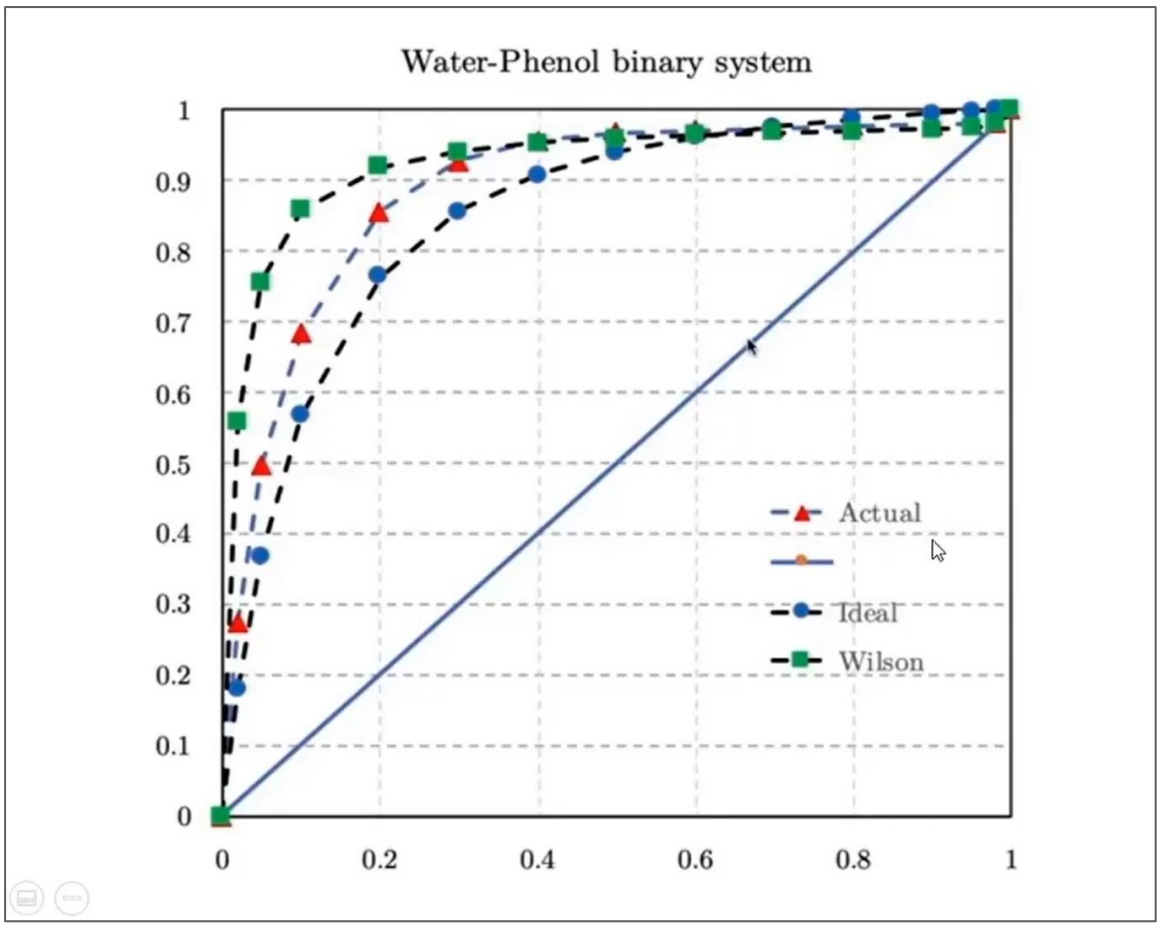
For Wilson Properties, select WILSON under property method and obtain the required results and graph. Other quantities are similar to water phenol system in ideal properties which does not need changes.



| Figure |

COMPARISION OF ACTUAL, IDEAL AND WILSON GRAPH

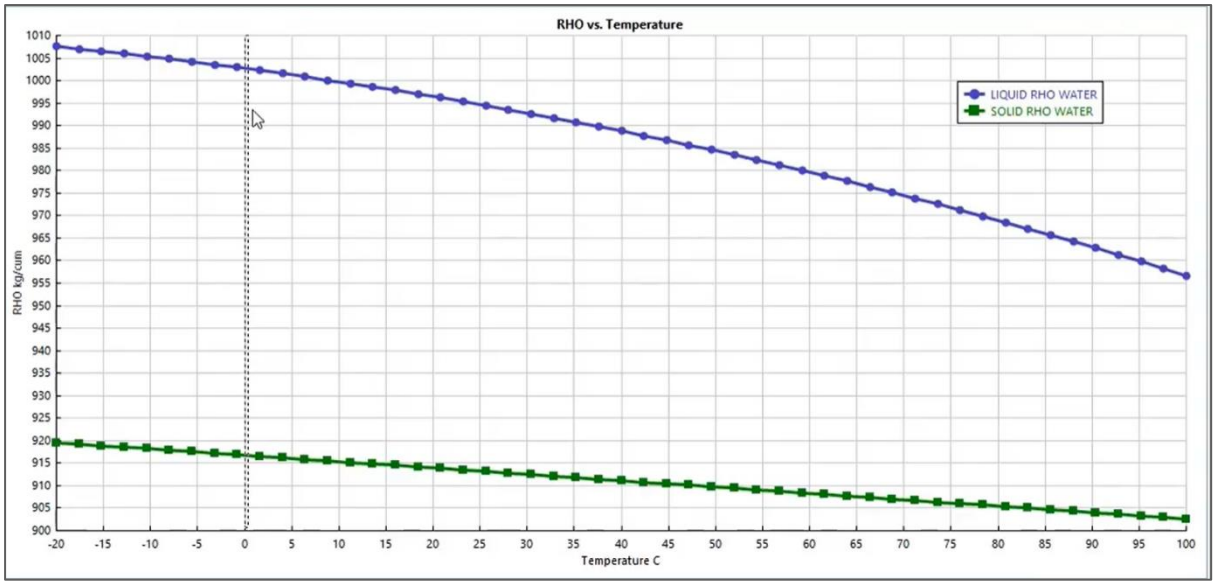
After obtaining the respective individual graphs for Ideal and Wilson Properties, we compare them with the actual properties graph all together in one place and observe the following.



| Figure |

PURE SYSTEM ANALYSIS OF WATER

Now we will be doing a pure system analysis of water in Aspen Plus. For this, we need to select a pure component, i.e. water with property type as Thermodynamic, RHO. The lower limits and upper limits are automatically filled by the system. We have to select NRTL property method and run the analysis under 1.01325 bar pressure to obtain the required results and graph.



| Figure |

Green curve represents solid phase and blue curve represents liquid phase. The data given by Liquid RHO Water (Blue curve) is analysed when the temperature is lesser than 0. Whereas, the date given by Solid RHO Water (Green curve) is analysed when the temperature is greater than 0.

BINARY ANALYSIS IN ASPEN PLUS

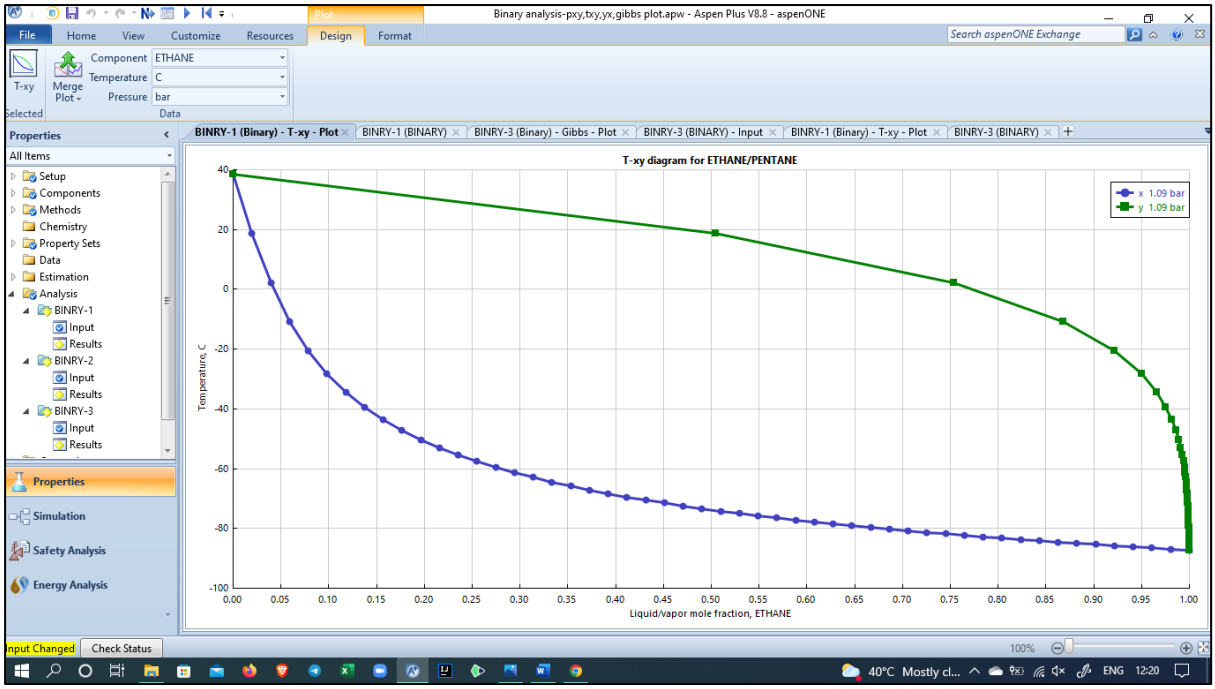
Before working on Aspen Plus, let us know what is Peng-Robinson Equation of state. **Peng-Robinson Equation of State** is an equation which can be applied for mixtures of gases. This equation expresses fluid properties in terms of the critical properties and acentric factor of each species involved.

The Peng-Robinson Equation of State:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V^2 + 2bV - b^2}$$

PENG-ROBINSON UNDER CONSTANT PRESSURE (T – xy Plot)

We are going to do Binary analysis under Peng-Robinson property method in Aspen Plus to obtain the required graph for components Ethan and Pentane under constant pressure condition.



| Figure | Done in Aspen Plus

Vapor Liquid Equilibrium (VLE) exists in the region between the y (green curve) and x (blue curve) curves. It can be represented by drawing a Tie Line.

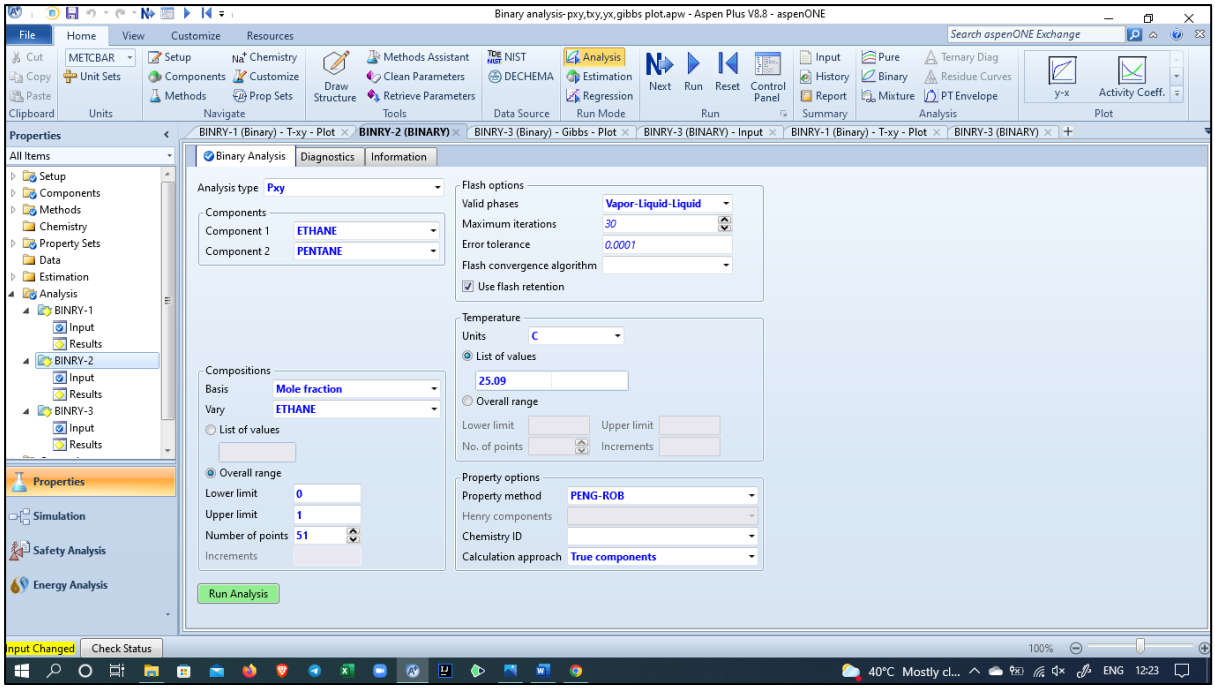
Tie Line is a line that represents VLE at a particular temperature and pressure. Below the blue curve, liquid will exist and above the green curve, vapor will exist. Any point on the blue curve is called Bubble Point and any point in the green curve is called Dew Point.

Bubble Point refers to the pressure at which the first flow of air through a liquid saturated fabric occurs.

Dew Point is the temperature to which air must be cooled to become saturated with water vapor, assuming constant air pressure.

PENG-ROBINSON UNDER CONSTANT TEMPERATURE (P – xy Plot)

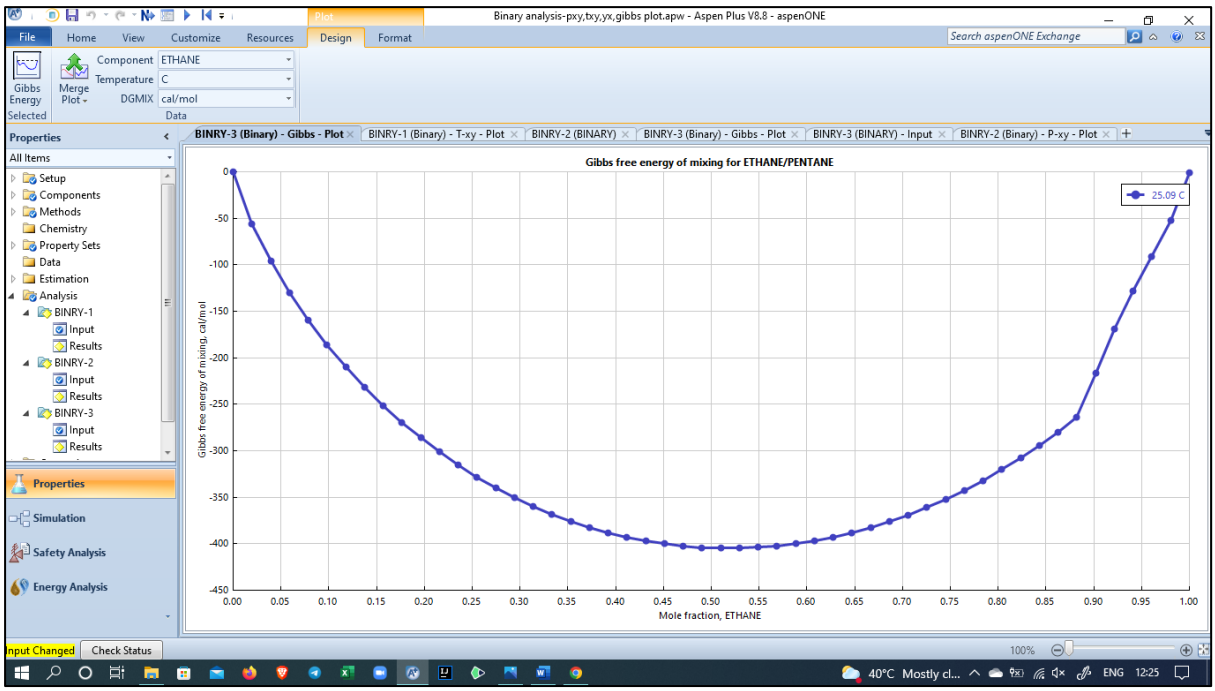
We are going to do Binary analysis under Peng-Robinson property method in Aspen Plus to obtain the required graph for components Ethan and Pentane under constant temperature condition.



| Figure | Done in Aspen Plus

PENG-ROBINSON USING GIBB'S FREE ENERGY

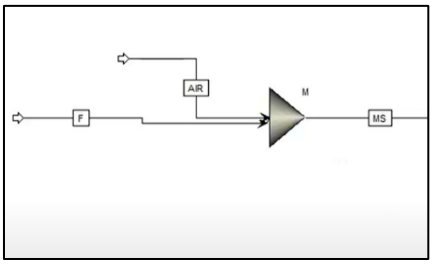
Now, using property method Peng-Robinson, we will obtain a Gibb's Free Energy graph for Ethane and Pentane in Aspen Plus.



| Figure | Done in Aspen Plus

MIXER IN ASPEN PLUS

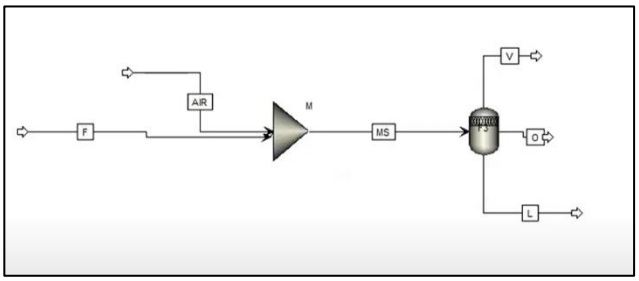
Mixers play an important role in many different production processes, at the beginning or at the end. Some processes require several feed streams to be properly mixed before a reaction is commenced in a reactor. Other processes require that final products are blended together. Mixers serve to achieve both of these roles.



Suppose, a problem is given and we need to find the data of the outlet stream. We are given three components water, toluene and NAPHT-01 as feed stream at constant temperature 25°C and pressure 1.5 atm. The total flow rate is 1000 kg/hr. The mole fraction of water, toluene and NAPHT-01 are 0.56, 0.26 and 0.18. Another stream of air at same temperature and pressure has total flow rate of 500 kg/hr.

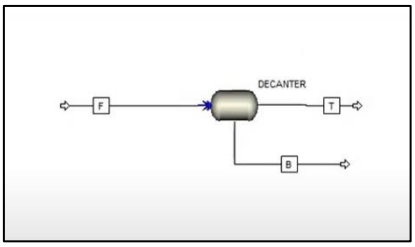
Firstly, we make a flow diagram which has the feed and air as inlet streams connected to the mixer. The outlet stream coming out of the mixer is MS. Next, we put the inlet data in the state variables and composition section of a mixer. We repeat the steps for both feed and air separately. Then we click of next and finally run it in Aspen Plus. To see the results, we click on MS, then on Stream Results to see the output results.

FLASH SEPARATORS IN ASPEN PLUS



Flash separation is a technique used to separate the gas and liquid species in a stream that is at vapor-liquid equilibrium (VLE). Either the species can be at VLE before entering the separator, or the separator may add or remove heat to bring the system to VLE. **Flash separators** are used in flash separation. There are two types of flash separators in Aspen Plus: Flash2 and Flash3. **Flash2** has two outlets: a vapor outlet at the top and a liquid outlet at the bottom. **Flash3** has three outlets: vapor outlet at the top, liquid outlet at the bottom and light liquid outlet at the middle. Flash separators depend on VLE.

DECANTER IN ASPEN PLUS



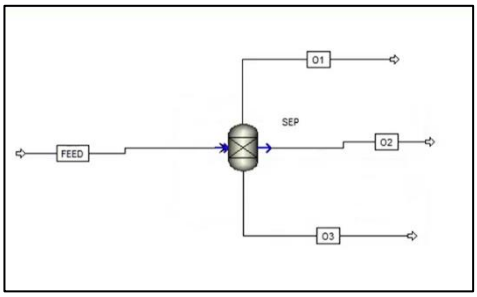
A decanter centrifuge separates solids from one or two liquid phases in one single continuous process. This is done using centrifugal forces that can be well beyond 3000 times greater than gravity. **Decater depends on density.**

Suppose, we are given two components P-XYLENE and water of mass fraction 0.5 each as input. The inlet temperature and pressure are 30 degree celcius and 1 atm, respectively. Total flow rate is 2000 kg/hr. It is also given, that the decanter is operating at a temperature and pressure of 40 degree celcius and 1 bar.

Now, to get the outlet results, we select a decanter in Aspen Plus and enter the input and decanter operating conditions in the respective boxes. Once we run it, we get the results and can see that lighter product Xylene is coming out from the top of the decanter whereas heavy product is coming out from the bottom of the decanter.

If we select key component as xylene, we will get more fraction of xylene in the outlet stream.

SEPARATORS IN ASPEN PLUS



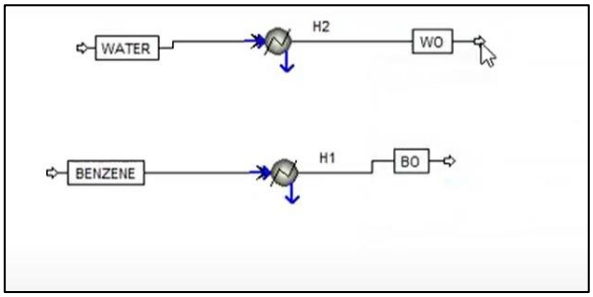
A vapor-liquid separator is a device used in industrial applications to separate a vapor-liquid mixture into its constituent phases.

It is a 3-phase vertical separator which has three outlets flowing from top, middle and bottom. While working on Aspen Plus, we just have to specify the inlet temperature, pressure and flow rate. For the outlet, we need to specify separatly. At the end, we also have to define outlet stream conditions and then run them to get the results.

EXCHANGERS

Heat exchangers are used to thermally process materials, and can be employed to heat or cool a range of products in applications such as food processing, chemical processing, energy production, and waste management. Heat exchangers play an important role in maximizing the use of energy in many of these heating and cooling applications by transferring heat efficiently and recovering heat for reduced energy use and environmental impact.

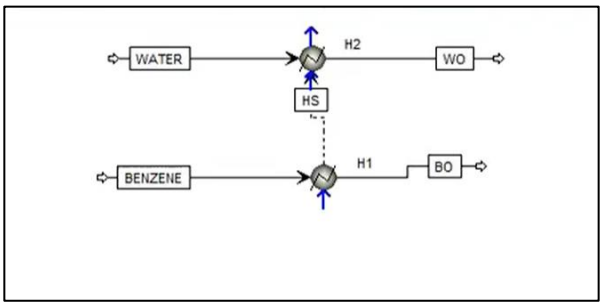
HEATER



Heater is a simple model whose main purpose is to calculate duty requirements for changing the temperature of a stream. They are used to provide heat for a process or can serve as reactor which provides heat of reaction.

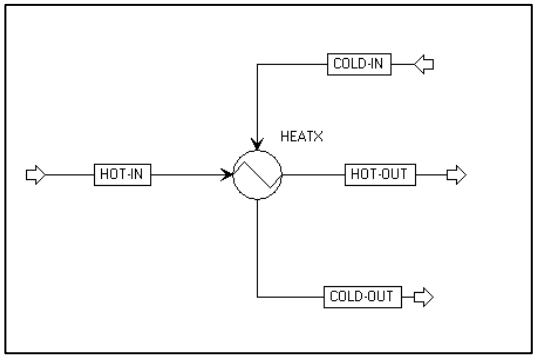
A heater in Aspen Plus works under specified pressure and duty. Specification of feed is done in the state variables section which consist of temperature, pressure, total flow basis, total flow rate, etc. We also need to specify the composition of the feed. In the figure, water is heated by heater 2 to get water outlet. Similarly, benzene is heated by heater 1.

Exchange of heat between two heaters



In this type of configuration, exchanging of heat takes place between the two heaters. We are only asked to add one parameter (either pressure, temperature, temperature change or pressure drop) in the heater specification section.

HEATX



A second kind, HeatX, is a more rigorous heater. HeatX requires that there be two streams that pass through the heat exchanger. One stream is to be heated/cooled and the other stream performs the heating/cooling. For example, the two streams are one made of benzene, which is at temperature 30 degrees celsius (cold inlet) and water at temperature 300 degrees celsius (hot inlet). It has to be passed through a heatX heat exchanger of duty 10kW. All these can be done in Aspen Plus. First, designing is done, then rating, and lastly, simulation.

To build the system in Aspen, we will need two feed streams, two product streams, and one HeatX type heat exchanger. Our flowsheet should look something like the figure. Hot-out stream and cold out stream will have water and benzene, respectivily.

DISTILLATION

Distillation is simply defined as a process in which a liquid or vapor mixture of two or more substances is separated into its component fractions of desired purity, by the application and removal of heat. It is heating the liquid to form vapor and then cooling it to get back the liquid. It is used to separate components of a mixture containing two miscible liquids that boil without decomposition and have sufficient difference in their boiling points.

Some important terms that we need to know:

Stripping section: The section in a distillation column located below the feed point, in which the less volatile component or components in the mixture undergoing separation increase in concentration towards the bottom of the column as the more volatile component or components are stripped out.

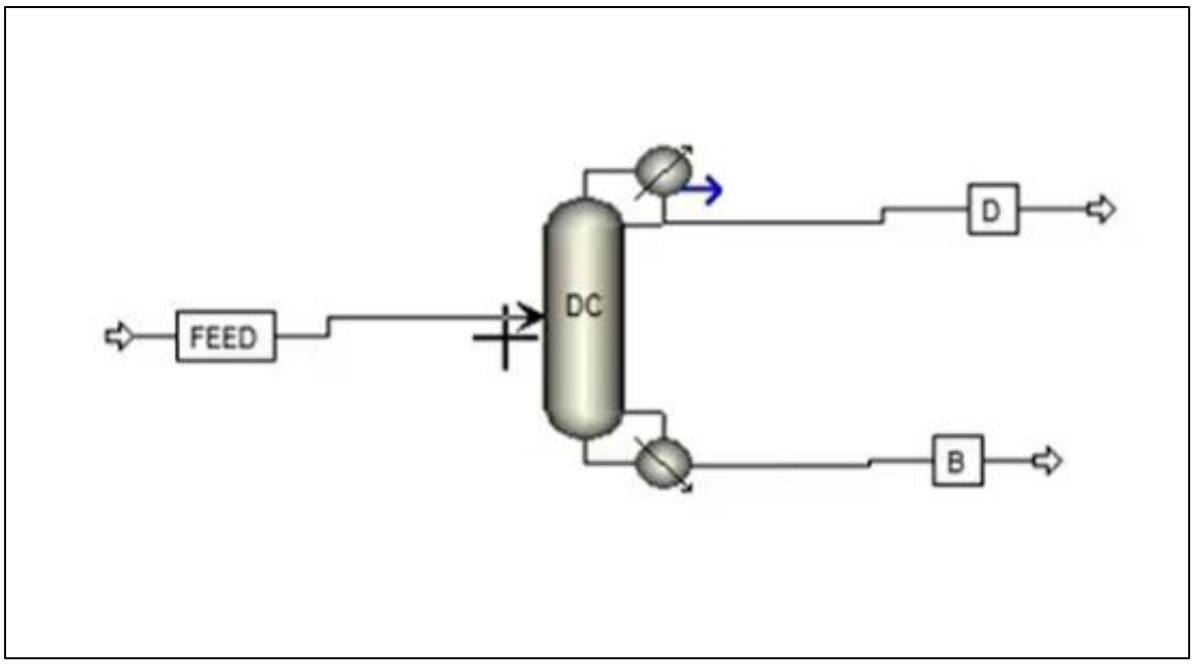
Enriching section: The portion of a counter current contractor above the feed point in which an upward-moving, product-rich stream from the stripping column is further purified by counter current with a downward-flowing reflux stream from the overhead product-recovery vessel.

Reflux ratio: The reflux ratio is defined as the ratio of the liquid returned to the column divided by the liquid removed as product.

We will notice a number of distillation column options in Aspen Plus. We will mainly discuss about DSTWU and RadFrac here.

DSTWU

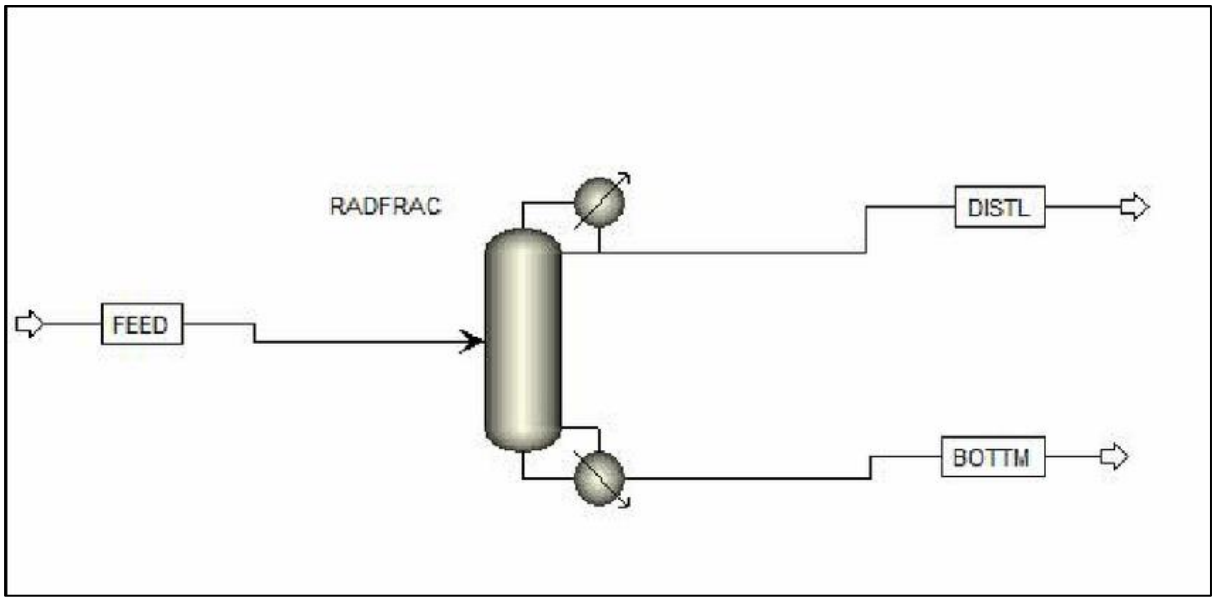
The DSTWU unit operation is designed for single feed, two product distillation processes. For a specified product recovery (both light and heavy), the DSTWU column first estimates the minimum number of stages and the minimum reflux ratio, and then it calculates the either the required reflux ratio or 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.



| Figure |

RADFRAC

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. **It gives more tuned results.** 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.



| Figure |

REACTOR MODELLING

Reactor modelling is a very useful tool in the design and scale-up of commercial reactors, enabling prediction of the system behaviour under different operating conditions without the need for expensive and time-consuming experimentation.

REACTOR MODELS

There are 7 built-in reactor models, RSTOIC, RYIELD, REQUIL, RGIBBS, RPLUG, RCSTR and RBATCH, in Aspen Plus™. RPLUG, RCSTR and RBATCH are rigorous models for plug flow, CSTR and batch reactors, respectively.

REACTORS		
BALANCED BASED	EQUILIBRIUM BASED	KINETICS BASED
RYield	REquil	RBatch
RStoic	RGibbs	RPlug & RCSTR

| Figure |

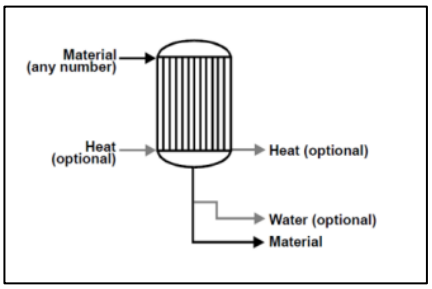
RSTOICH should be used in cases where the stoichiometry is known but the reaction kinetics is either unknown or negligible. If both, the reaction kinetics and stoichiometry is unknown RYIELD should be incorporated into the simulations. For single phase chemical equilibrium or simultaneous phase and chemical equilibrium calculations the reactor model of choice should be either REQUIL or RGIBBS. REQUIL bases its calculations on simultaneous solution of stoichiometric chemical and phase equilibrium calculations whereas RGIBBS solves its model by minimizing Gibbs free energy.

All reactor models except RPLUG and RBATCH can have any number of material feed streams. These streams are mixed internally.

Model	Stoichiometry	Kinetics	Rigorous	Feed
RSTOIC	Yes	No	No	Any
RYIELD	No	No	No	Any
REQUIL	No	No	No	Any
RGIBBS	No	No	No	Any
RBATCH	Yes	Yes	Yes	1
RCSTR	Yes	Yes	Yes	Any
RPLUG	Yes	Yes	Yes	1

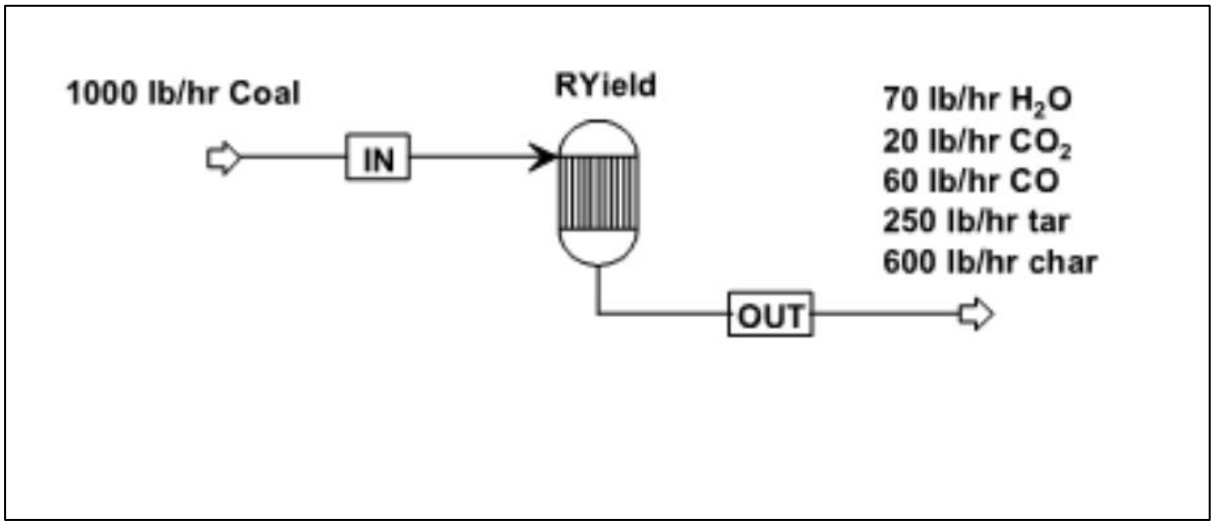
| Figure |

RYIELD REACTORS



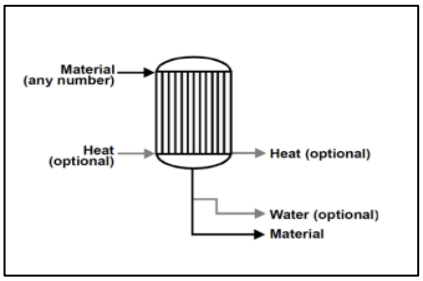
RYield reactors require a mass balance only with no atom balancing. It is used to simulate reactors in which inlets to the reactor are not completely known but outlets are known. An example can be to simulate the furnace.

RYield, performs the calculations based on the yield. The block takes streams as shown in the figure to the right. This block does not require exact information about the stoichiometry or kinetics. The output of the reaction is defined based on the yield in the Setup. The yield is defined as mole or mass of each component per total mass input to the block. Inert components can be defined in the same form and will not be included in the yield calculations. No heat of reaction can be calculated here because the stoichiometry of the reaction is not known. Another option to enter the yield is through the component mapping option. In this form, the combination (lumping) or breaking (de-lumping) of reactants (with their weight fraction) to form products is input for each material.



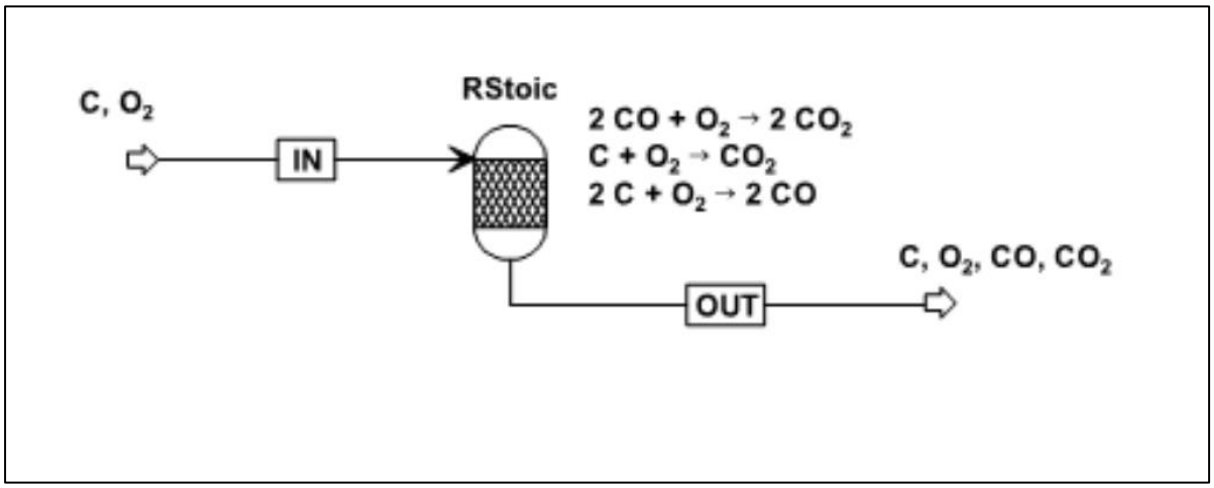
| Figure |

RSTOIC REACTORS



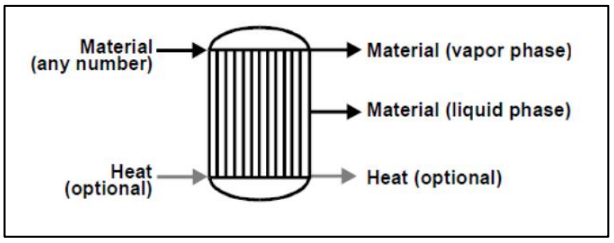
RStoic reactor model requires both an atom and a mass balance. It is used in situations where the stoichiometry is known but both the equilibrium data and the kinetics are either unknown or unimportant. The block must have one or more feed streams, one required output stream. Optional connections are the water decant and input and output heat streams. The connectivity for this block is shown in the figure to the right. It can also specify or

calculate heat of reaction at a reference temperature and pressure.



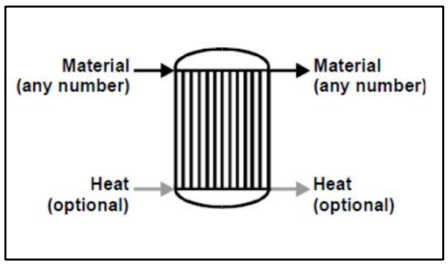
| Figure |

REQUIIL REACTORS



When one or more reactions involved are equilibrium reaction, the REquil block can be used. The block requires knowledge of the reaction stoichiometry, and performs chemical and phase equilibrium reactions. Unlike the previous blocks, the REquil block has a vapor and liquid phase product streams (both are required). The only required information for this block is the output stream and the reaction. With this input, all the required calculations are made based on thermodynamics calculations.
These reactors do not take reaction kinetics into account. It allows individual reactions to be at a restricted equilibrium. REquil computes combined chemical and phase equilibrium by solving reaction equilibrium equations. It cannot do a three-phase flash. These reactors are mostly useful when there are many components, a few known reactions, and when relatively few components take part in reactions.

RGIBBS REACTORS



The fourth block provides reaction calculations without the need for detailed stoichiometry or yield. The calculations are based on minimizing the Gibbs energy for the system. The block takes one or more input and one or more output

streams, and an optional heat input and/or output stream.

RGibbs is useful when reactions occurring are not known or are high in number due to many components participating in the reactions. A Gibbs free energy minimization is done to determine the product composition at which the Gibbs free energy of the products are at a minimum. This is the only Aspen Plus block that will deal with solid-liquid-gas phase equilibrium.

RCSTR & RPLUG REACTORS

When rigorous simulation of reactors is needed, the RCSTR and RPlug are used. These two blocks perform simulation of ideal reactors operated under specific conditions.
RCSTR reactors are used when reaction kinetics are known and when the reactor contents have same properties as outlet stream. It allows for any number of feeds, which are mixed internally. Three product streams are allowed – vapor, liquid1, liquid2 or vapor, liquid and free water. It can model equilibrium reactions simultaneously with rate – based reactions.

RPlug reactors are those reactors which can handle only rate-based reactions. A cooling system is allowed in this type of reactor. Reactor length and diameters are important when it comes to this reactor.

RBATCH REACTORS

RBatch reactors are those reactors that can handle rate-based kinetic reactions only. Any number of continuous or delayed feeds are allowed. Whenever one uses a RBatch reactor, it is a must to provide one of the following: stop criteria, cycle time or result time. Holding tanks are used to interface with steady-state streams of Aspen Plus.

REACTION RATE

The reaction rate or rate of reaction is the speed at which a chemical reaction takes place, defined as proportional to the increase in the concentration of a product per unit time and to the decrease in the concentration of a reactant per unit time. Reaction rates can vary dramatically.

POWER – LAW RATE EXPRESSION

A common form for the rate equation is a power law. The constant k is called the rate constant. The exponents, which can be fractional, are called partial orders of reaction and their sum is the overall order of reaction.

$$\textbf{Rate} = k\,\Pi[\text{concentration}_i]^{\text{exponent}_i}$$

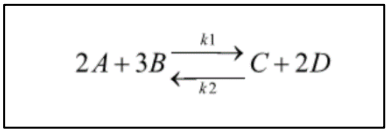
$$\boldsymbol{k = (Pre - exponential\ Factor)\left(\frac{T}{To}\right)^{n} exp\left(-\frac{Activation\ Energy}{R}\left[\frac{1}{T} - \frac{1}{To}\right]\right)}$$

If reference temperature, T_o is not specified, k is expressed as:

$$\boldsymbol{k = (Pre - exponential\ Factor) * T^{n} exp\left(-\frac{Activation\ Energy}{RT}\right)}$$

POWER – RATE EXPRESSION EXAMPLE

Reaction:



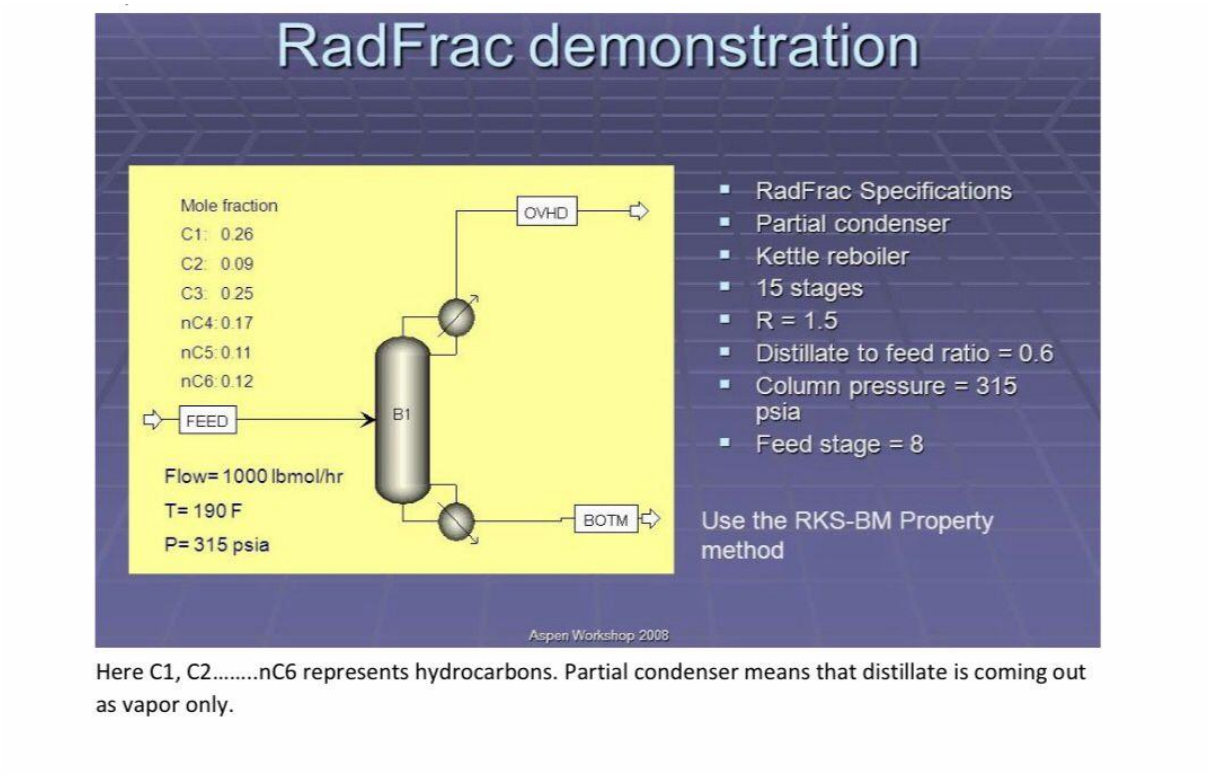
Forward Reaction: (Assuming the reaction is 2nd order in A)

The definition of forward reaction for any chemical change would be about the reactants reacting and producing the products on the right side of the arrow. Any forward reaction would move to the right side where products or product is formed.

Reverse Reaction: (Assuming the reaction reaction in 1st order in C and D)

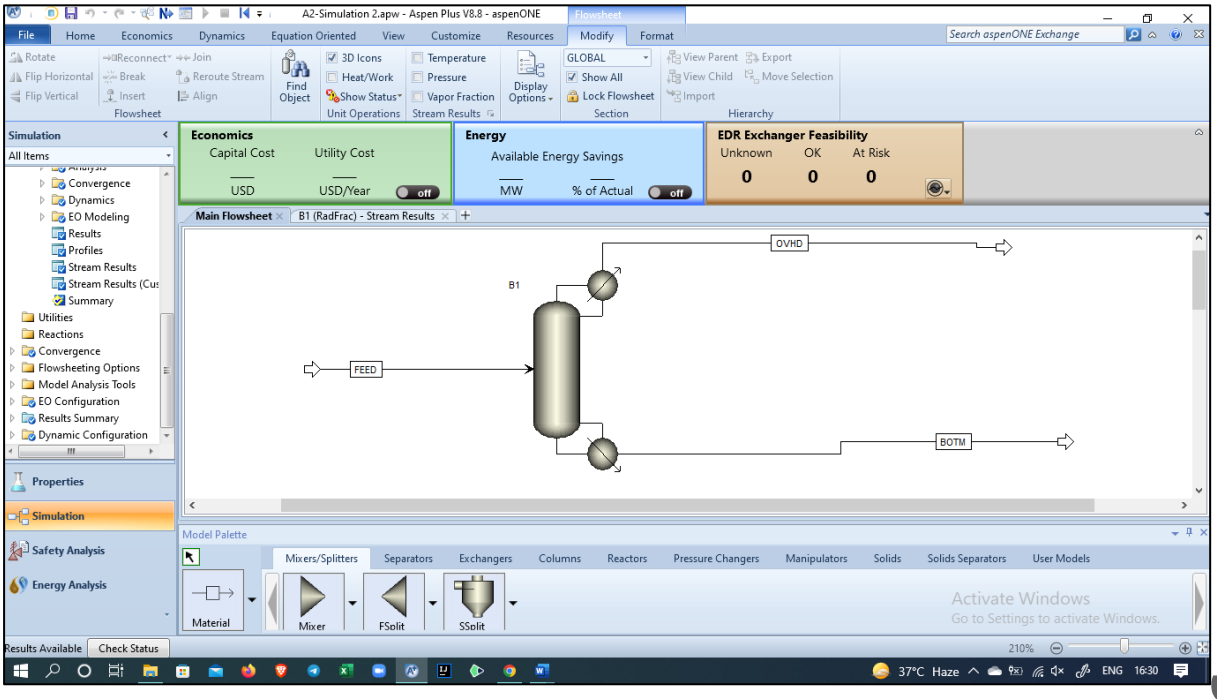
A reversible reaction is a reaction in which the conversion of reactants to products and the conversion of products to reactants occur simultaneously. A and B can react to form C and D or, in the reverse reaction, C and D can react to form A and B. This is distinct from a reversible process in thermodynamics.

RADFRAC DEMONSTRATION

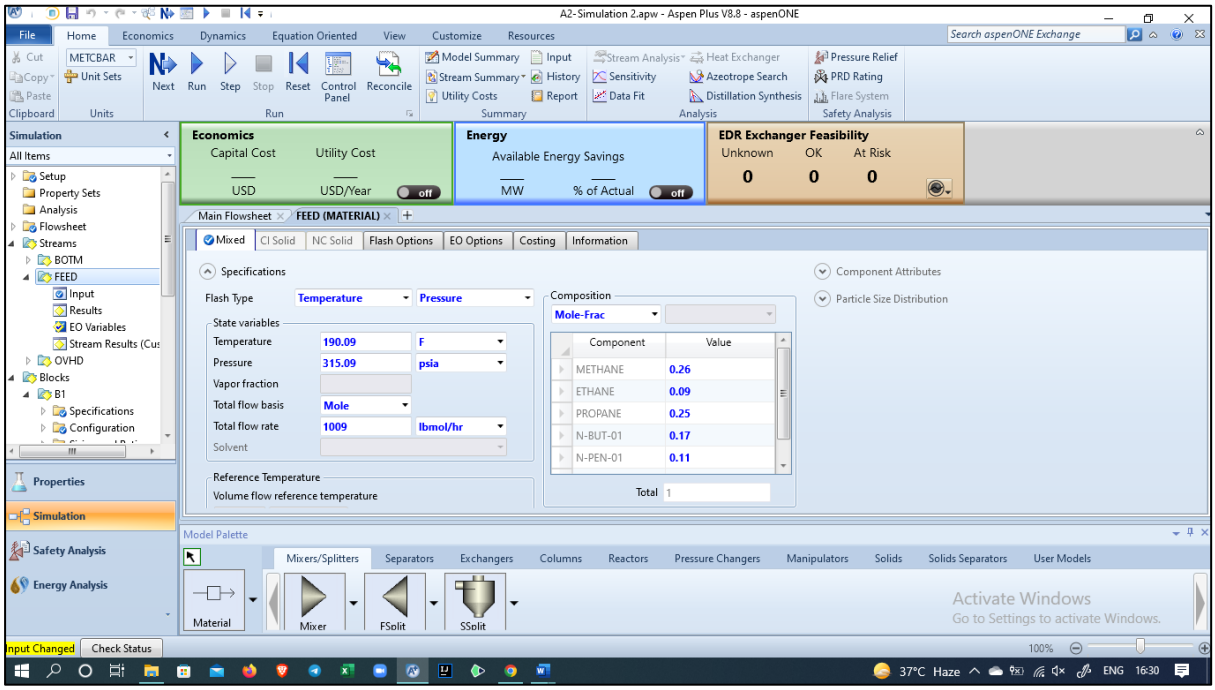


Here C1, C2.....nC6 represents hydrocarbons. Partial condenser means that distillate is coming out as vapor only.

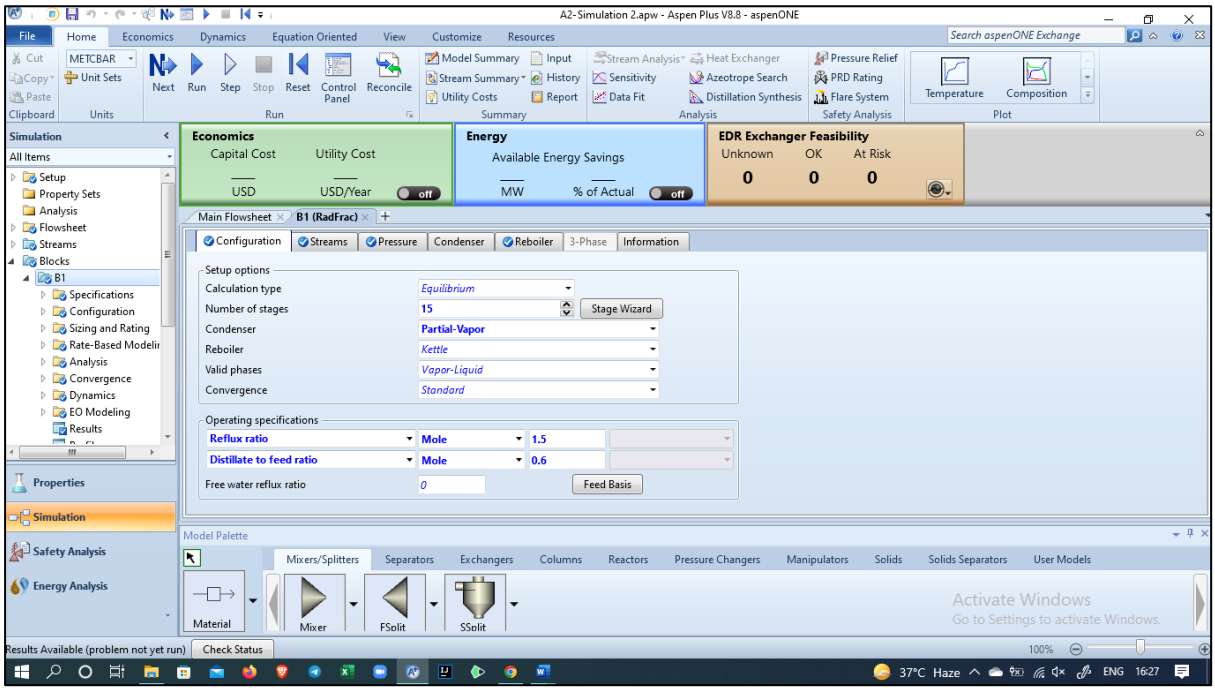
Here, we will be performing a RADFRAC demonstration on Aspen Plus. We will specify the given inputs in the given problem to come up with the required stream table. Firstly, we make the flow diagram with feed as input to the RADFRAC distillation column.



Now we have to set the components in Aspen Plus. In this problem, the components are methane, ethane, propane, n-butane and n-pentane with mole fraction of 0.26, 0.09, 0.25, 0.17 and 0.11.



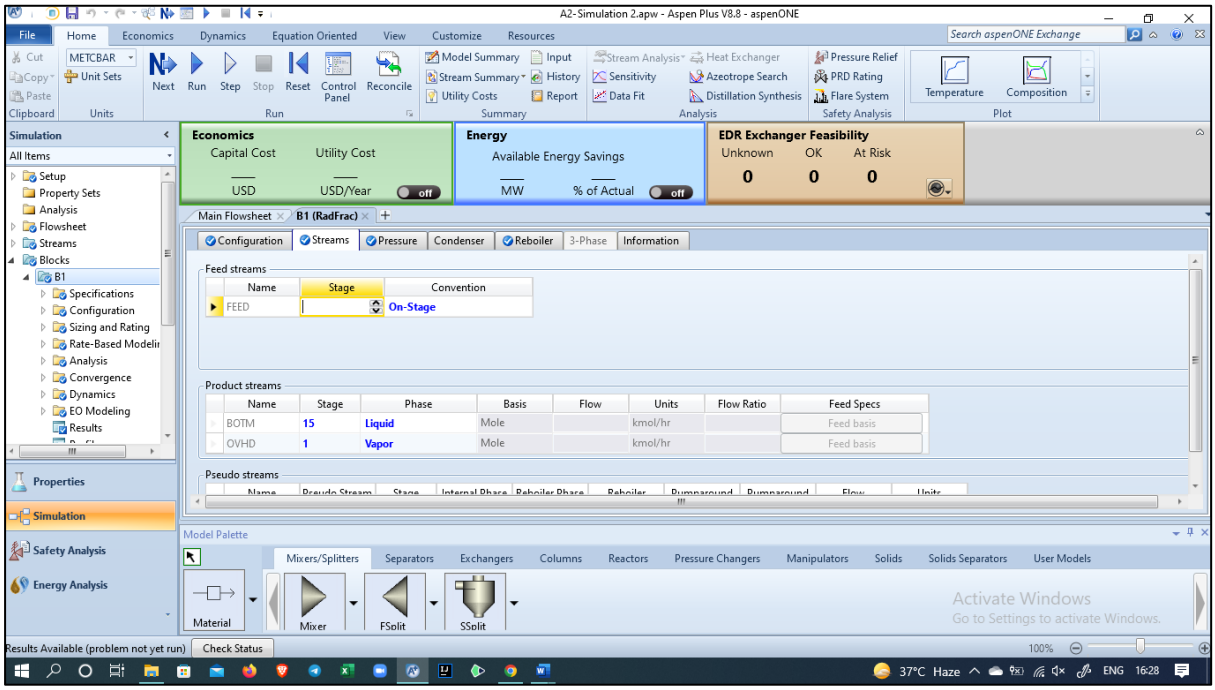
Feed Specification: Here, we need to input the required information in their respective blocks. The temperature is 190.09 F, pressure is 315.09 psia and total flow rate of feed is 1009 lbmol/hr.



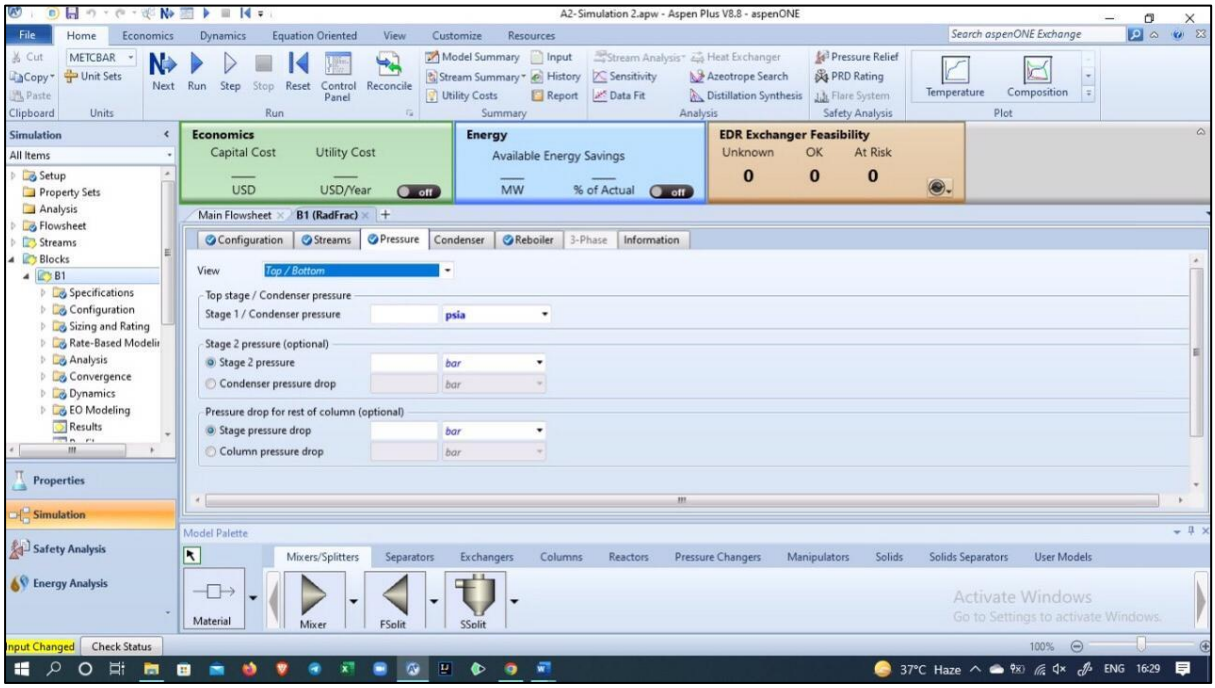
RadFrac Configurations: Now we have to set the RadFrac configurations. It involves setting the number of stages (which is 15 for this problem) for the process to take

place, setting the reflux ratio (which is 1.5 for this problem) and distillation to feed ratio (which is 0.6 for this problem).

Reflux ratio is defined as the ratio of the liquid returned to the column divided by the liquid removed as product.



Next, we will set the stages for individual streams.



Then we will set the condenser pressure as 315.09 psia. And then run it for the final time to get the stream results.

Stream Table:

Heat and Material Balance Table				
Stream ID		FEED	BOTM	OVHD
From			B1	B1
To		B1		
Phase		MIXED	LIQUID	VAPOR
Substream: MIXED				
Mole Flow	kmol/hr			
METHANE		118.9954	7.25686E-5	118.9954
ETHANE		41.19072	.0172692	41.17345
PROPANE		114.4187	4.415138	110.0035
N-BUT-01		77.80470	73.38328	4.421416
N-PEN-01		50.34422	50.33316	.0110601
N-HEX-01		54.92096	54.92096	4.01031E-6
Total Flow	kmol/hr	457.6747	183.0699	274.6048
Total Flow	kg/hr	21080.63	12824.98	8255.644
Total Flow	l/min	6652.748	572.1874	4298.762
Temperature	C	87.82778	151.6098	23.34192
Pressure	bar	21.72469	21.75848	21.75848
Vapor Frac		.7025297	0.0	1.000000
Liquid Frac		.2974703	1.000000	0.0
Solid Frac		0.0	0.0	0.0
Enthalpy	cal/mol	-26863.15	-34508.18	-21561.61
Enthalpy	cal/gm	-583.2172	-492.5861	-717.1969
Enthalpy	cal/sec	-3.4152E+6	-1.7548E+6	-1.6447E+6
Entropy	cal/mol-K	-70.88079	-108.9178	-46.54566
Entropy	cal/gm-K	-1.538870	-1.554744	-1.548233
Density	mol/cc	1.14658E-3	5.33246E-3	1.06467E-3
Density	gm/cc	.0528118	.3735659	.0320078
Average MW		46.06028	70.05512	30.06373
Liq Vol 60F	l/min	675.1970	343.7085	331.4885