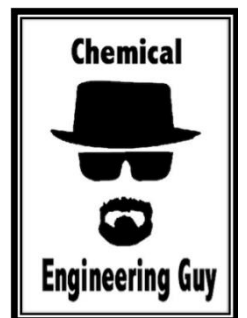


Aspen Plus® Getting Started!

Chemical Engineering Guy

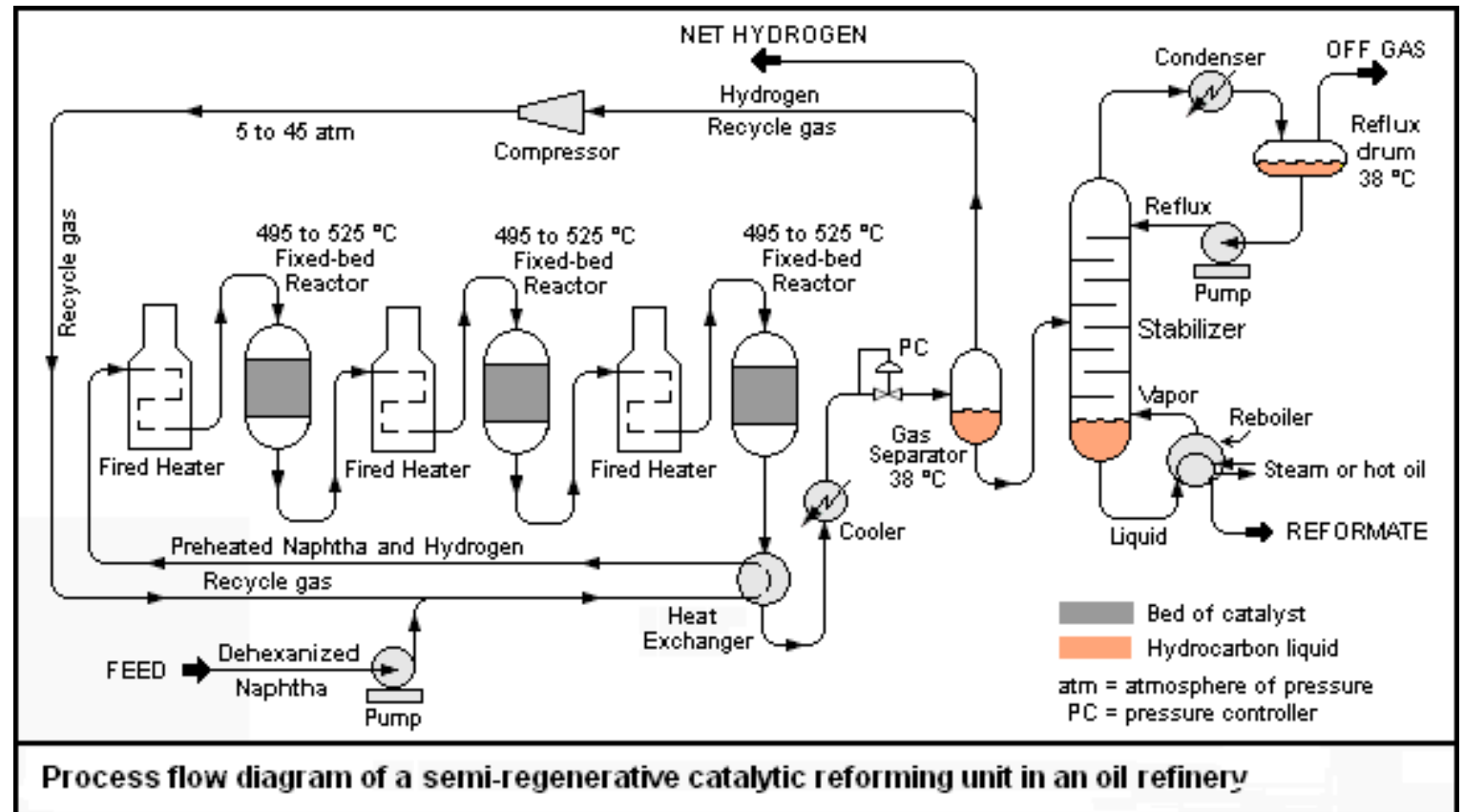
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Solve this!

Change:

- All T of Reactors
- Feed Composition
- No. of Plates in Distl. Col
- T of Heat Ex
- Gas Sep. T
- Compressor P
- Utility Costs



And this....



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Why Process Modeling/Simulation?

- Makes us easier/faster work
- Multiple and Simultaneous Simulations
- Different Real-Life Scenarios
 - Change on raw/feed materials scenario
- Pricing and Costs calculation
 - Raw Materials
 - Plant Cost
 - Utilities
- How it would behave under different conditions
 - High/Low Pressure
 - Humidity Changes
 - Temperature change (cool/warm days/seasons)



Which companies model?

- Mainly:
 - Petrochemical
 - Pharmaceutical
 - Fine chemicals
- Other commodities such as:
 - Sulfuric acids
 - Chlorine/Caustic industry
 - Solvents
 - Coatings
 - Many more...



Other Advantages...

- Excellent for your curriculum as an engineer
- Perfect for analytical/numerical minds
- Good for debugging and fixing “what if” scenarios



CONTENT INDEX

1. Introduction
2. Our Chemical Process!
3. Setting up the Physical Property Environment
4. Simulation Environment I – The Flowsheet
5. Simulation Environment II – Unit Operations
6. Running, Results & Analysis
7. Case Studies (A,B,C,D)
8. Conclusion



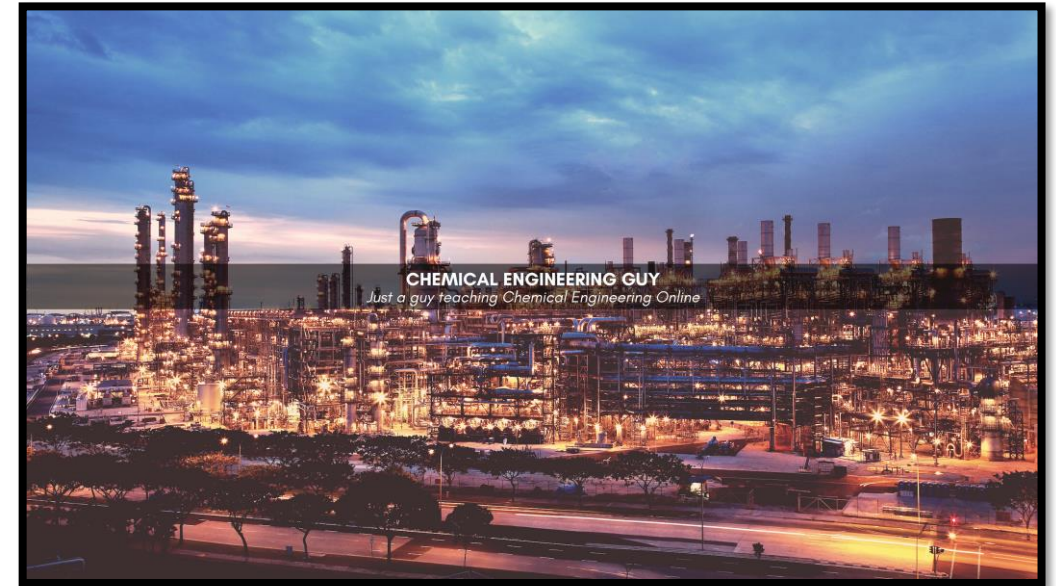
Course Objectives

- **Introductory Knowledge of Processes Modeling**
 - Setting the adequate Physical Properties
 - General Flowsheet Concepts
 - Basic Flowsheet “manipulation”
 - Common Unit Operations
 - Minimum Requirements to set up & run a Simulation
 - Analyze several changes in process conditions
 - Create an interest in Process Modeling



Contact

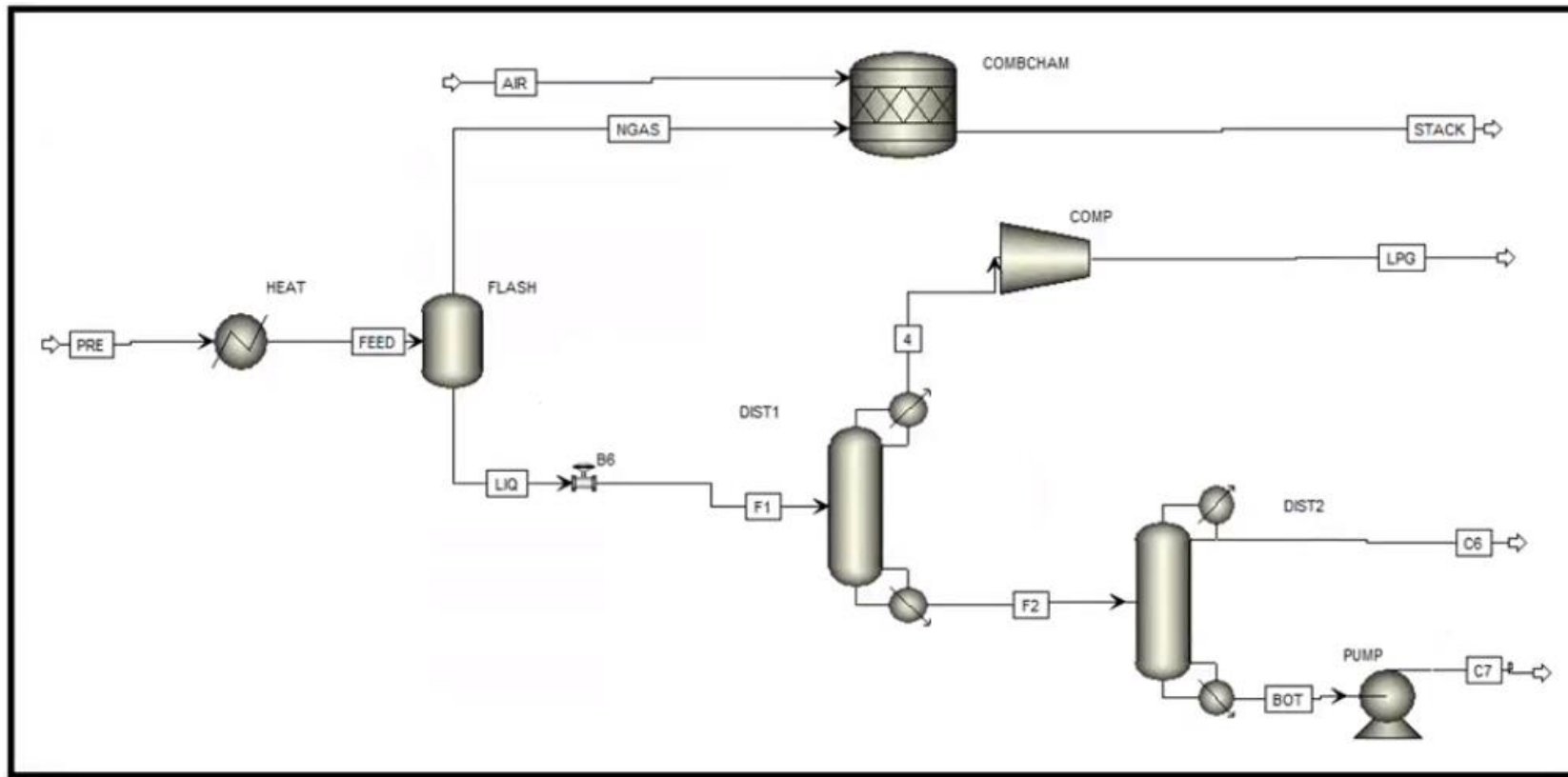
- Please contact me if required (doubts, questions, comments, suggestions)
 - Contact@ChemicalEngineeringGuy.com
- More courses...



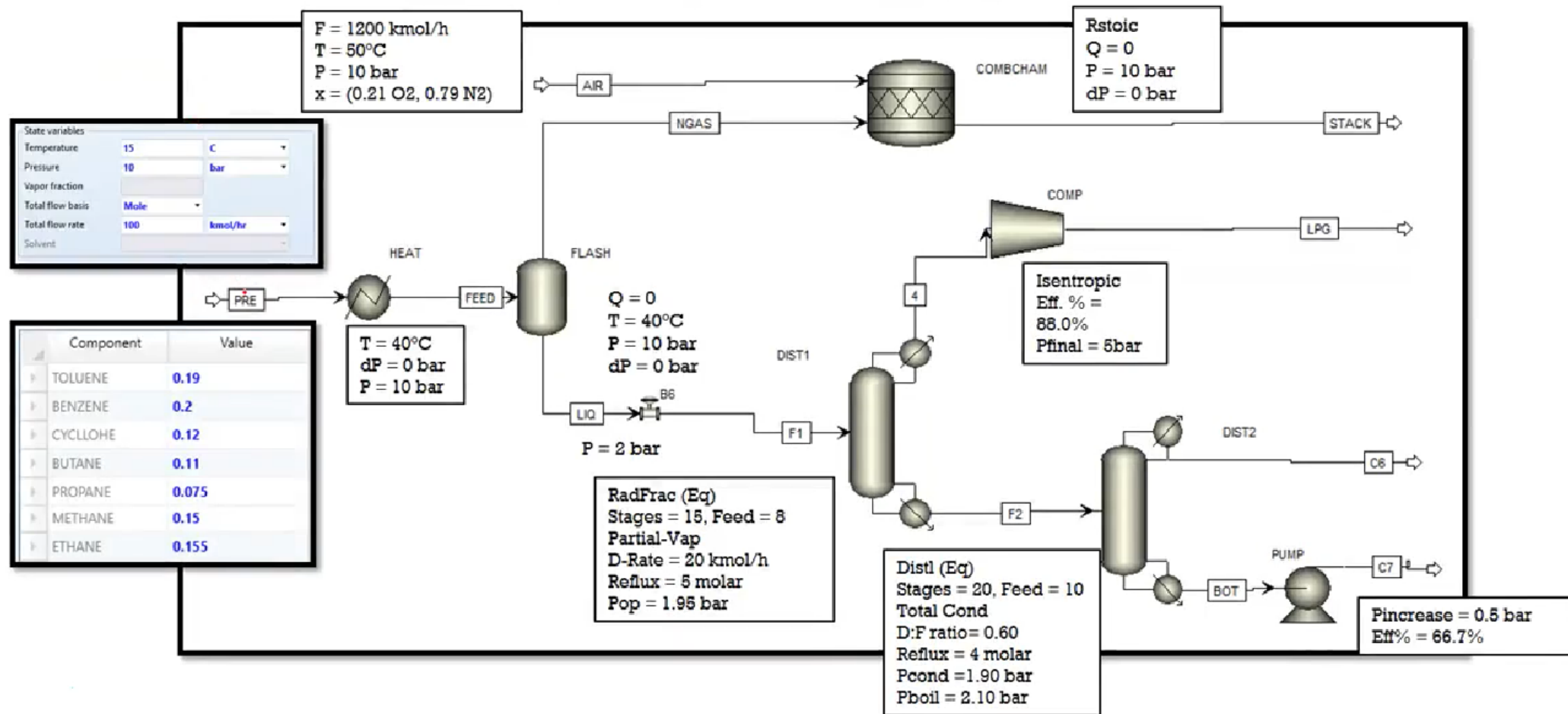
www.ChemicalEngineeringGuy.com



2. Our Chemical Process!



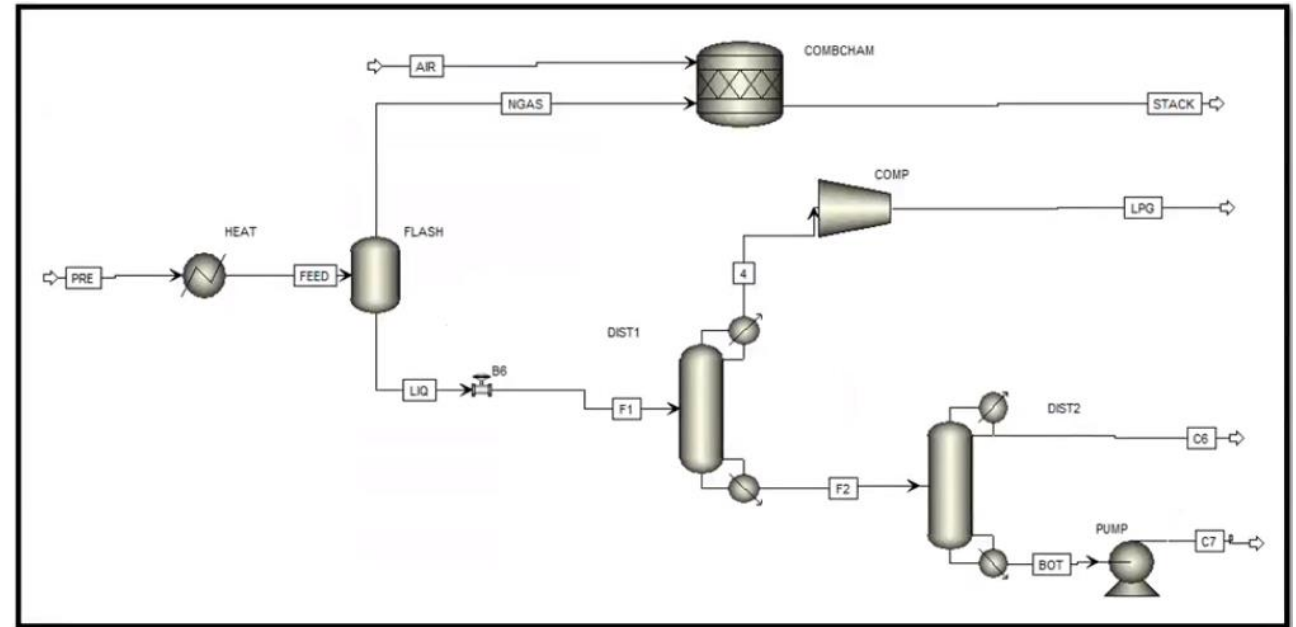
2. Our Chemical Process!



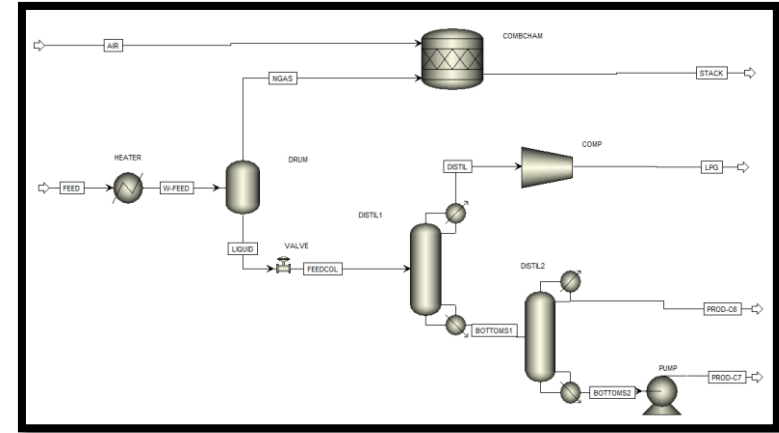
Conditions

- **Unit Operations**

- Heat Exchange
 - Heat Exchanger
- Reaction Kinetics
 - Combustion Chamber / Reactor
- Momentum
 - Pump
 - Compressor
- Separation Process
 - Flash Drum
 - Distillation Columns



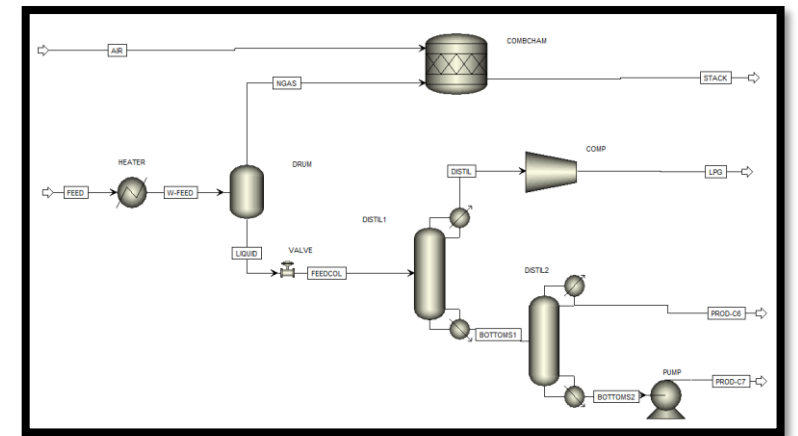
Problem Statement



- A hydrocarbon feed rich in aromatics is to be separated via a series of separation processes.
- It is sent from a previous plant at ambient temperature (15°C) and pressurized to 10 bar.
- A total of 100 kmol/h must be treated
- Most of the hydrocarbons must be recovered and the leftovers will be burnt in a combustion chamber.
- The combustion chamber will burn all hydrocarbons to form carbon dioxide. Assume 100% combustion. The air for combustion was previously adjusted to 50°C , 10bar. There is no pressure loss in the combustion chamber.
- The liquified section must be de-pressurized in order to continue treatment. It drops to 2 bar via a valve.



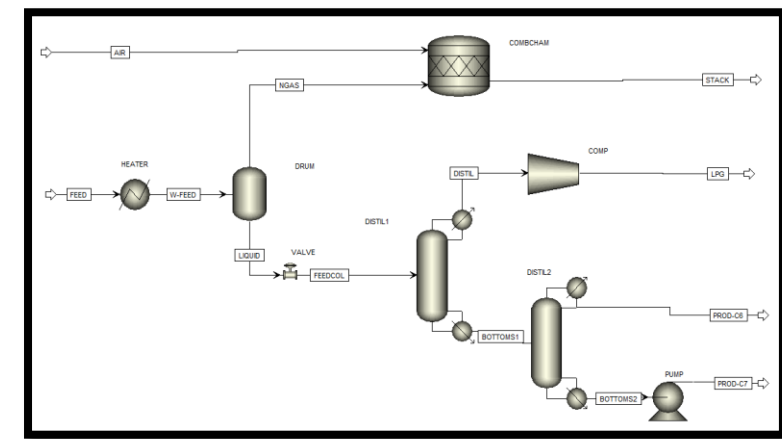
Problem Statement



- This stream is then fed to a Distillation Column.
 - It currently has a total of 15 trays.
 - Feed tray must be between 7 and 8.
 - Recommended operation is partial vapor in order to avoid an extra stage. Reflux
 - Ratio is set to 5 (molar) and the approx.
 - Pressure drop is unknown, but can be assumed to be low or negligible.
 - At least 20% of the feed must be recovered for further treatment
- The Distillate is to be treated in a following process. It must be compressed to 5 bar. We use a compressor with approx. 88% efficiency. It can be modeled as an isentropic compression.



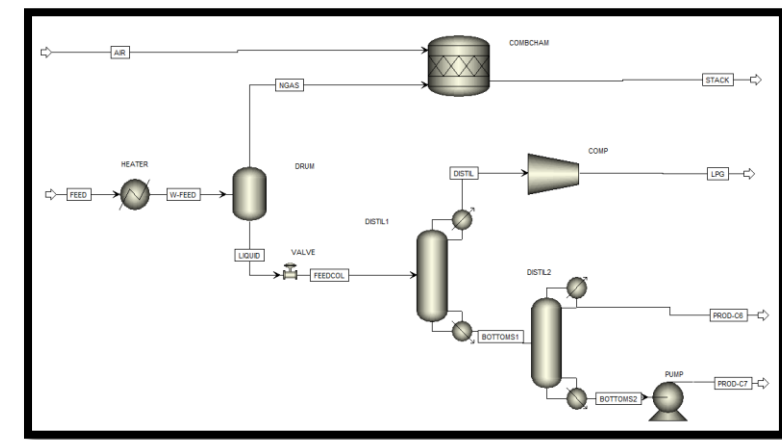
Problem Statement



- The bottoms of this column are not pure enough. Further distillation is required.
- The following column requires a total of:
 - 20 trays feeding in 50% approx.
 - It uses a total condenser since the distillate is required as a liquid
 - Recommended Distillate recovery is 60%
 - Reflux is set to 4 molar
 - The pressure drop is unknown, but current process has:
 - Condenser working at 1.90 bar
 - Reboiler working at 2.10 bar
- The distillate can be sent for storage
- The bottom must be further pressurized +0.5 bar in order to allow for pressure drop due to frictions. Efficiency of pump is 66.7%



Problem Statement



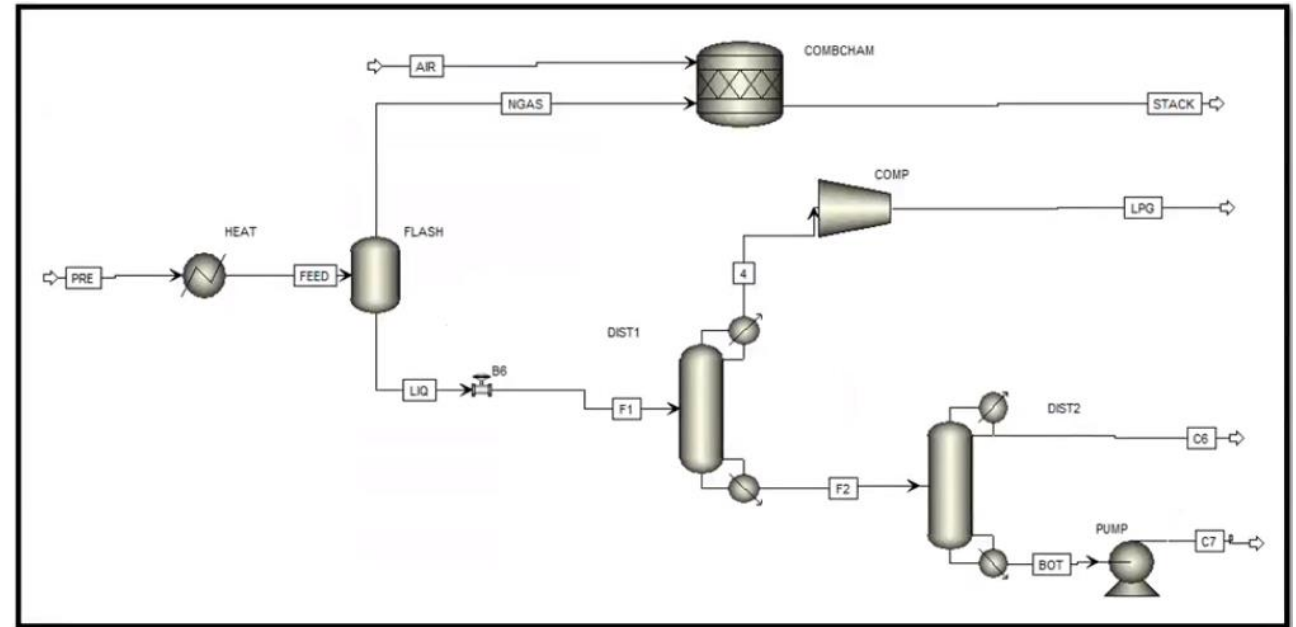
- Requirements:
 - Model the plant using Aspen Plus in Steady State
 - Verify Material/Energy Balances of the unit operations & processes
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 - Verify conditions such as T, P and Flow rates.
 - For specific unit operations, verify their relevant results
 - Heater → Heat duty
 - Combustion Chamber → T-max, Heat released by reaction
 - Compressor/Pump → Required Work
 - For the Columns → Reboiler & Condenser Duties



Conditions

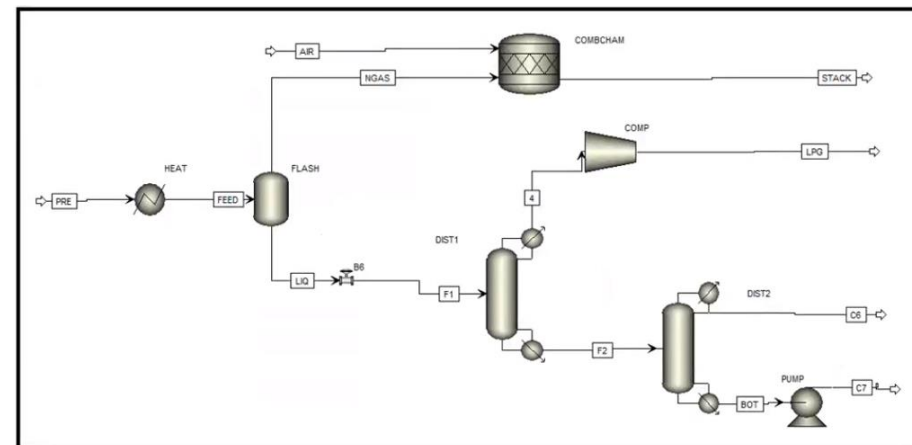
- **Unit Operations**

- Heat Exchange
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- Reaction Kinetics
 - Combustion Chamber / Reactor
- Momentum
 - Pump
 - Compressor
- Separation Process
 - Flash Drum
 - Distillation Columns



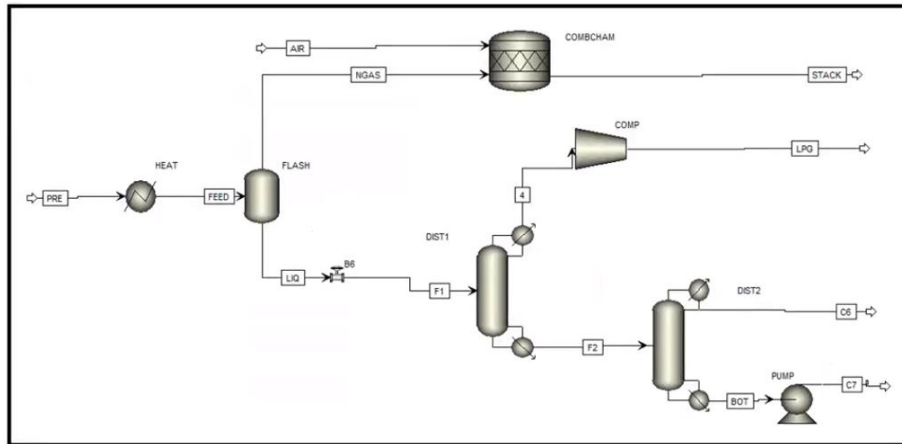
Examples

- Pipes



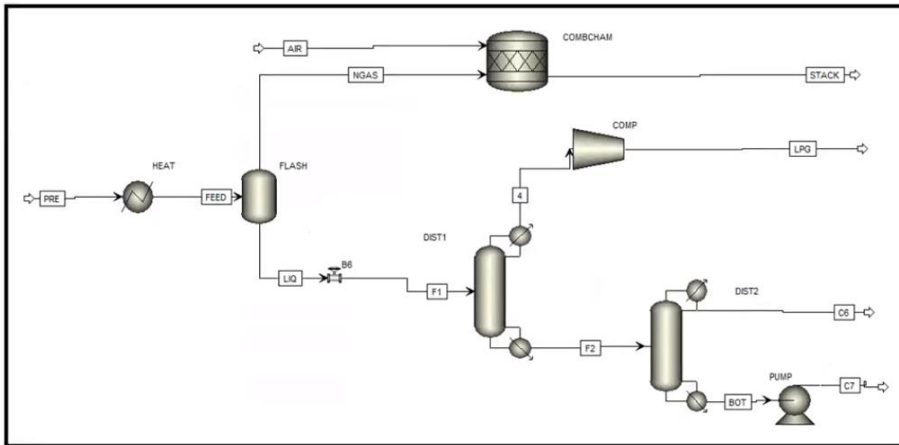
Examples

- Flash Tank:



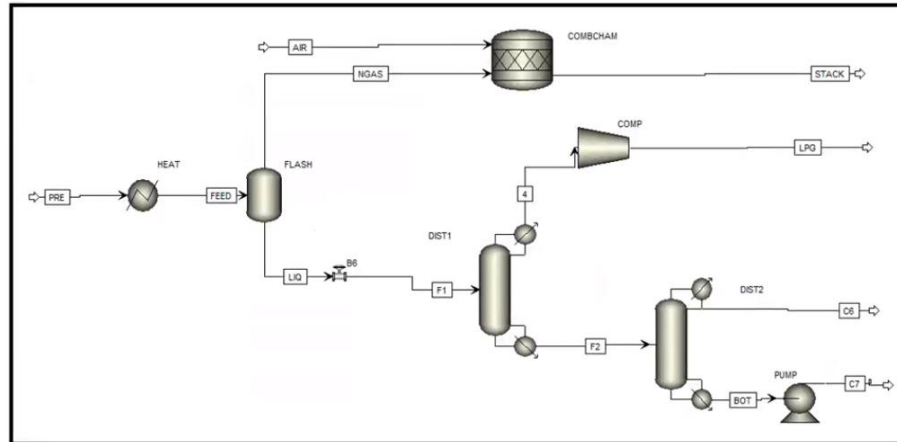
Examples

- Combustion Chamber / Reactor



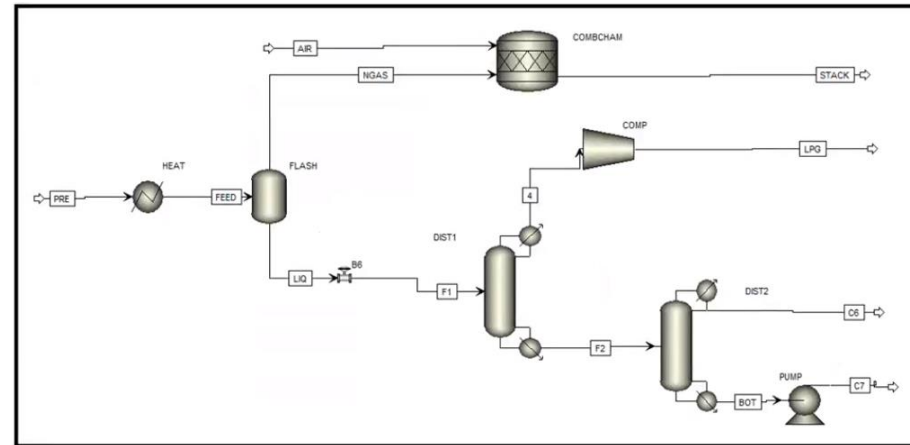
Examples

- Distillation Columns



Examples

- Compressor & Pump



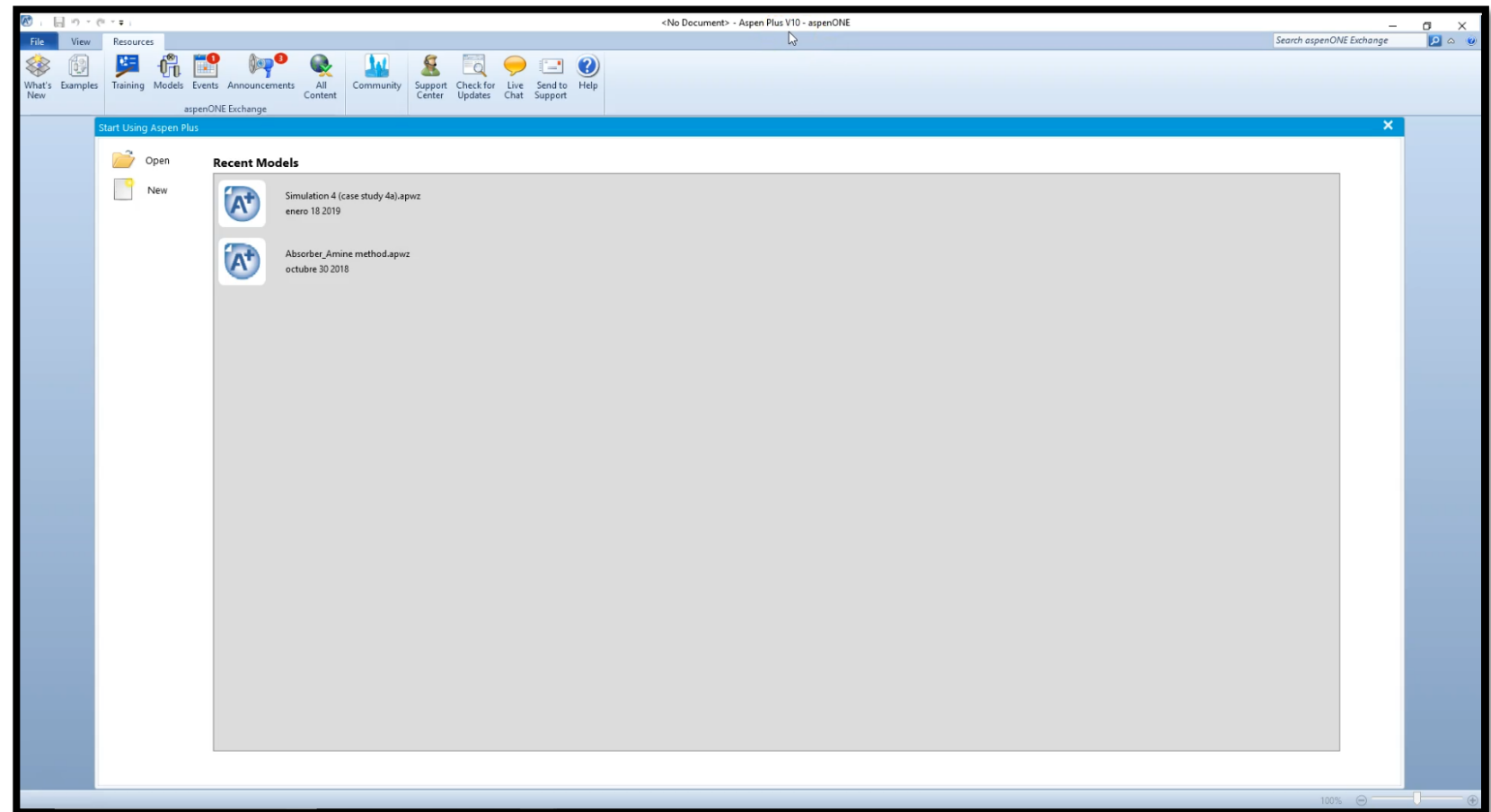
Resources

- PDF of Process diagram
- Spreadsheet with Unit Operations & Process conditions
- Spreadsheet with Component list & database



3. Physical Property Environment

- Landing Page



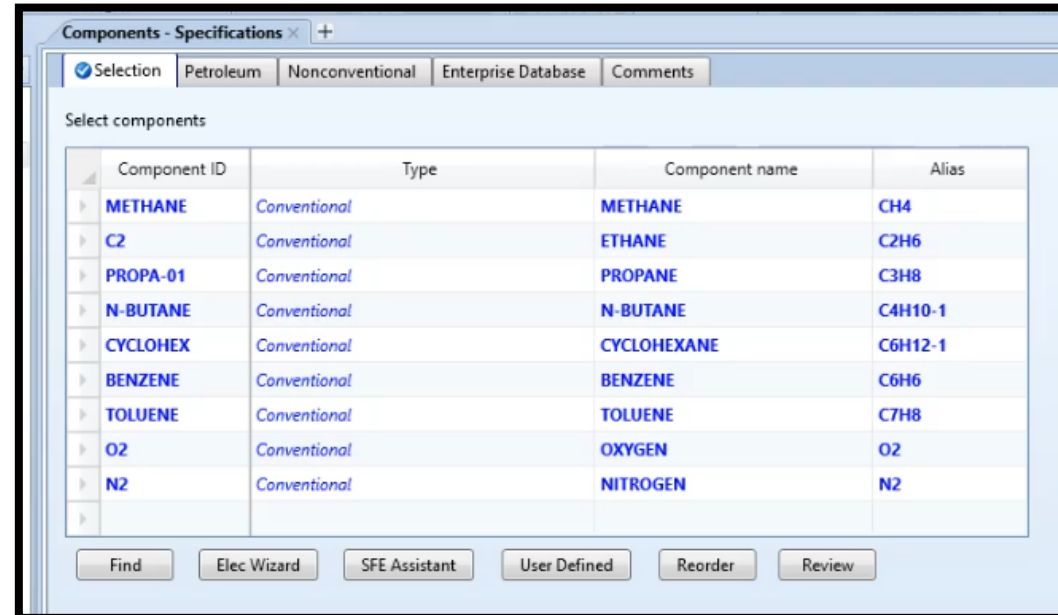
3. Physical Property Environment

- Min. Requirements:
 - Adding Components to the Component List
 - Selecting a Physical Property Method (Thermodynamic pack)
- If you want to further explore this environment →
 - **Aspen Plus - Physical Properties**
 - Different Types of Components
 - Methods (EOS, Activity, Mixed)
 - Modeling new/inexistent components
 - Physical & Chemical Property Analysis
 - Thermodynamic & Transport Properties



Adding Components

- Add the following compounds to the “Component List”
 - Methane
 - Ethane
 - Propane
 - N-Butane
 - Cyclohexane
 - Benzene
 - Toluene
 - Oxygen
 - Nitrogen



The screenshot shows a software window titled "Components - Specifications" with a tabbed interface. The active tab is "Selection". Below the tabs, there is a section labeled "Select components" containing a table with four columns: "Component ID", "Type", "Component name", and "Alias". The table lists several chemical components, all of which are of the "Conventional" type. At the bottom of the window, there are several buttons: "Find", "Elec Wizard", "SFE Assistant", "User Defined", "Reorder", and "Review".

Component ID	Type	Component name	Alias
METHANE	Conventional	METHANE	CH4
C2	Conventional	ETHANE	C2H6
PROPA-01	Conventional	PROPANE	C3H8
N-BUTANE	Conventional	N-BUTANE	C4H10-1
CYCLOHEX	Conventional	CYCLOHEXANE	C6H12-1
BENZENE	Conventional	BENZENE	C6H6
TOLUENE	Conventional	TOLUENE	C7H8
O2	Conventional	OXYGEN	O2
N2	Conventional	NITROGEN	N2

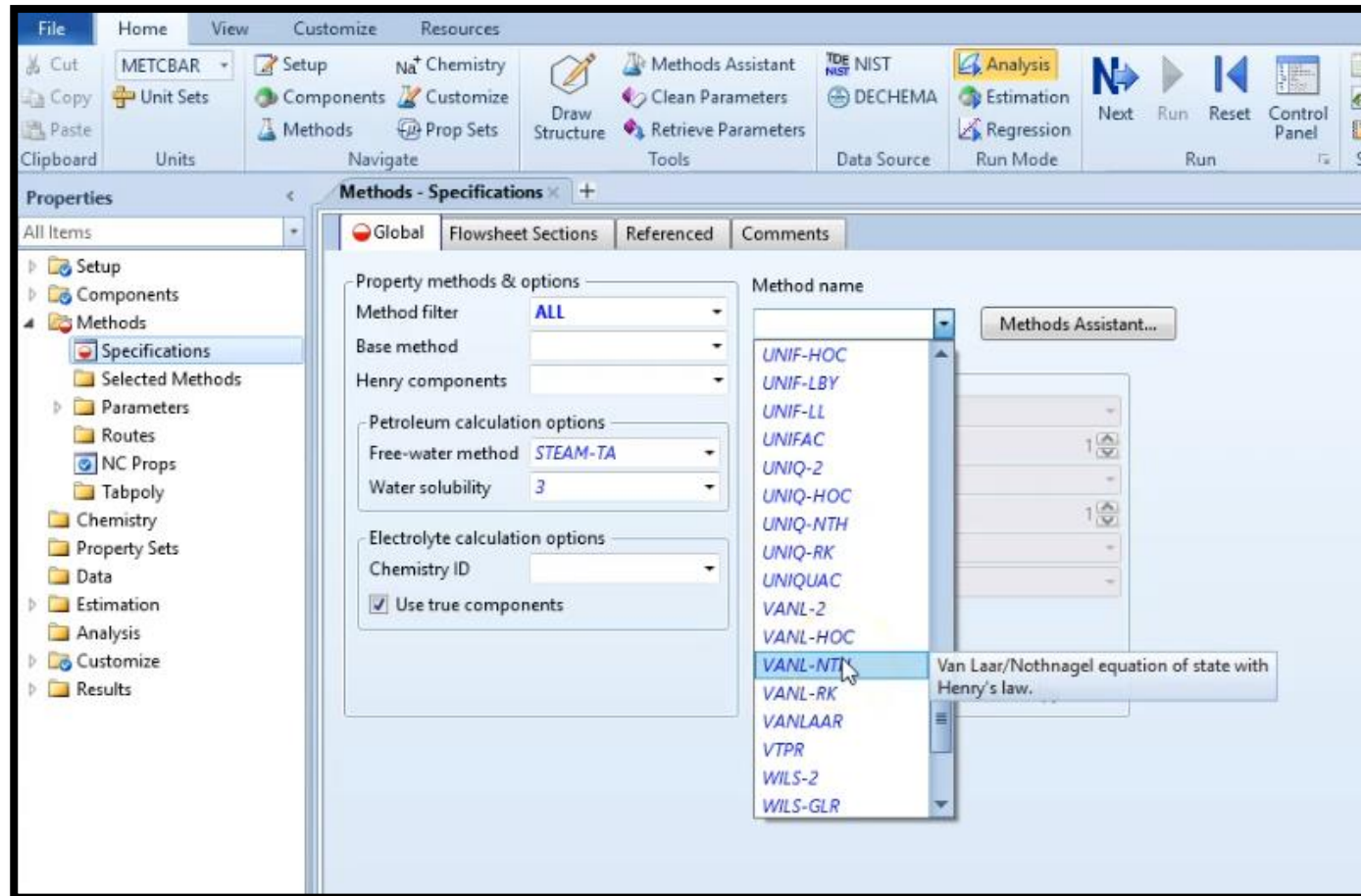


Choosing the Property Method

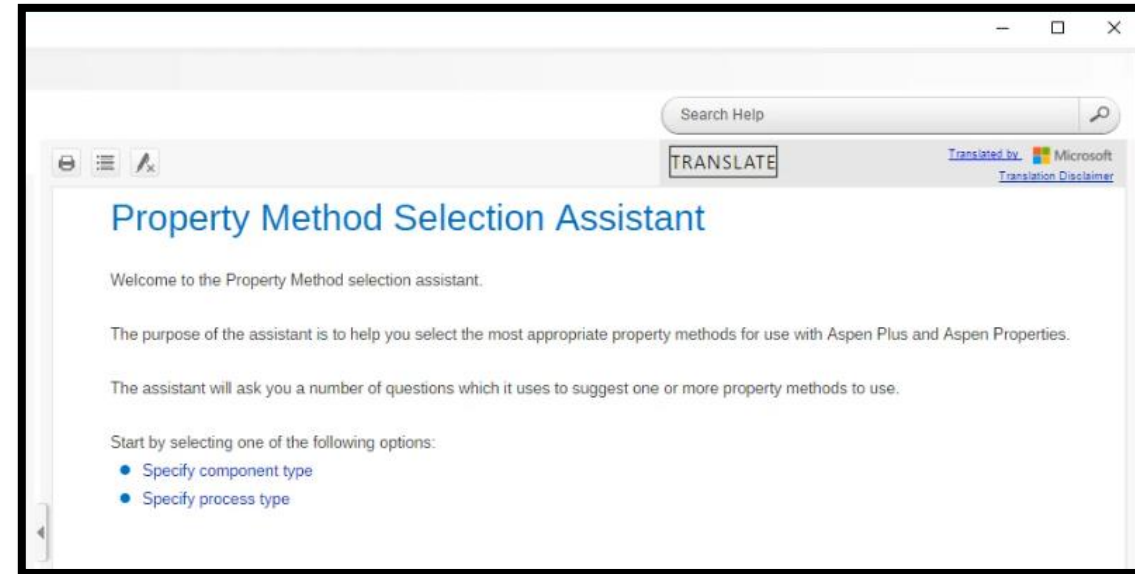
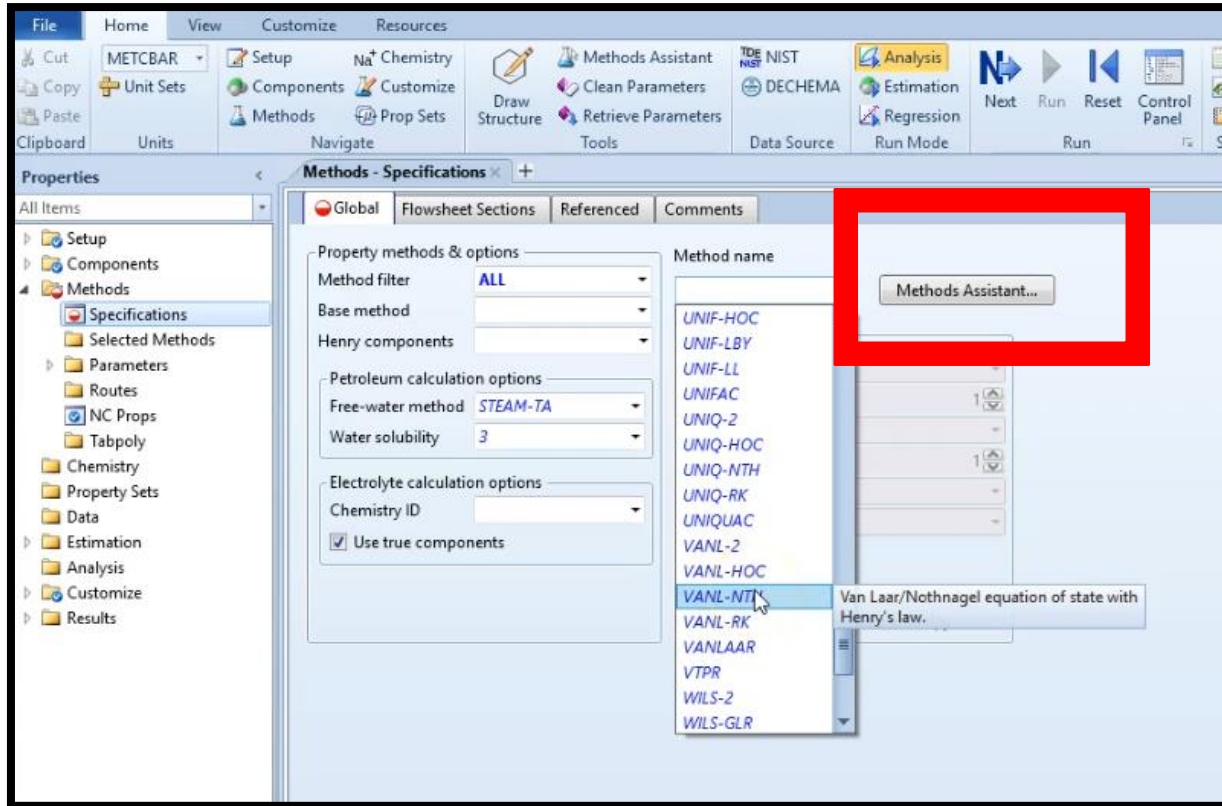
- Select Peng Robinson, as it is mostly non-polar system
 - Most models will be “set-up”
 - Pure substances Properties will be loaded
 - Binary Interactions are calculated
- Tip: Use the Method Assistant



Choosing the Property Method



Method Assistant...



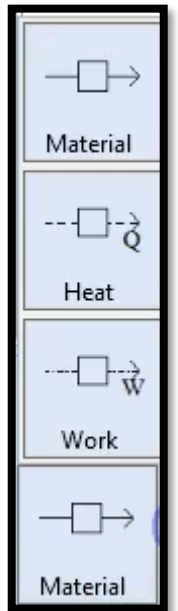
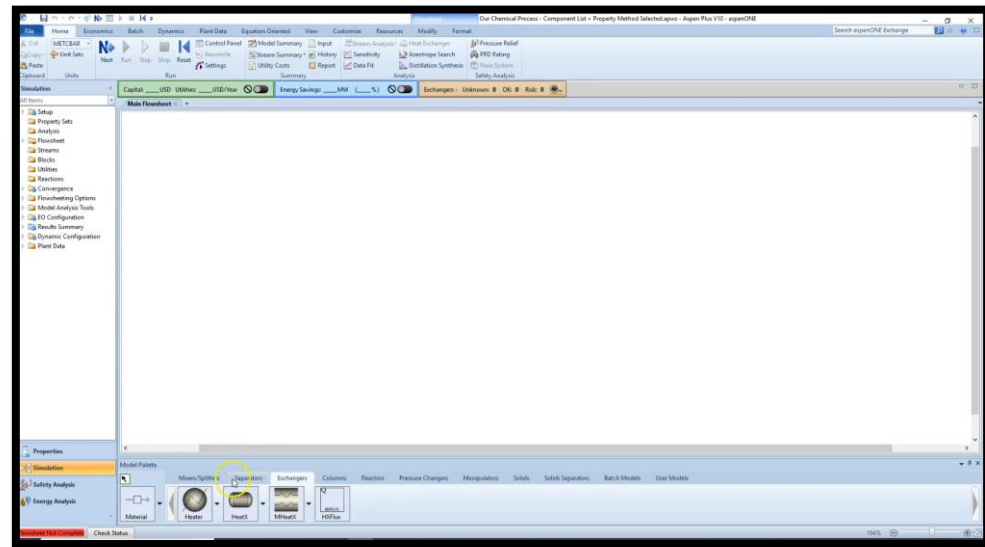
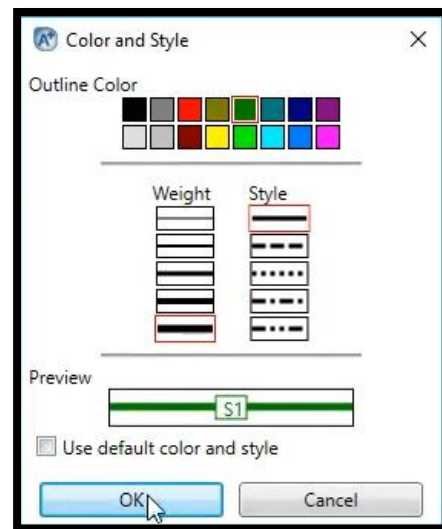
Simulation Environment I: The Flowsheet

- Get to know what is a flowsheet and how to manipulate it.
- Menus, Tool, Areas, etc...
- Important:
 - General Setup
 - Blocks: Unit Operations, Others
 - Streams (Material, Heat, Work)
 - Analysis tools



Simulation Environment I: The Flowsheet

- Manipulation of the Flowsheet:
 - Adding Unit Operations
 - Adding Material and Energy streams
 - Moving
 - Labeling
 - Rotating
 - Deleting
 - Copy and Pasting

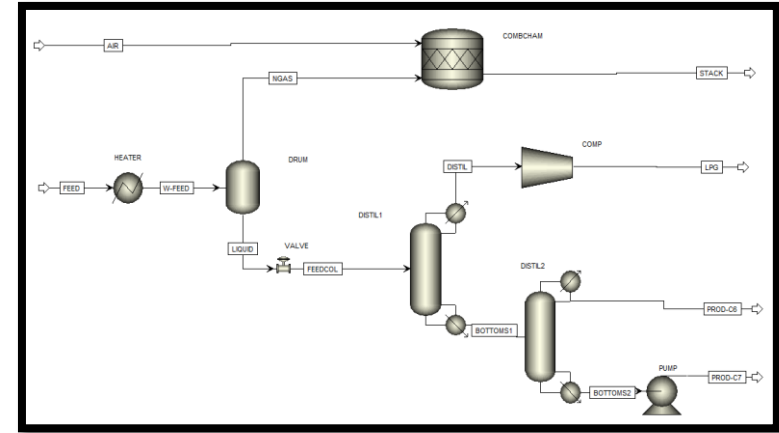


5. Simulation Environment II: Unit Operations

- Typical Unit Operations
- Adding UO
- Setting up
- Connecting streams
- Inlet/outlet



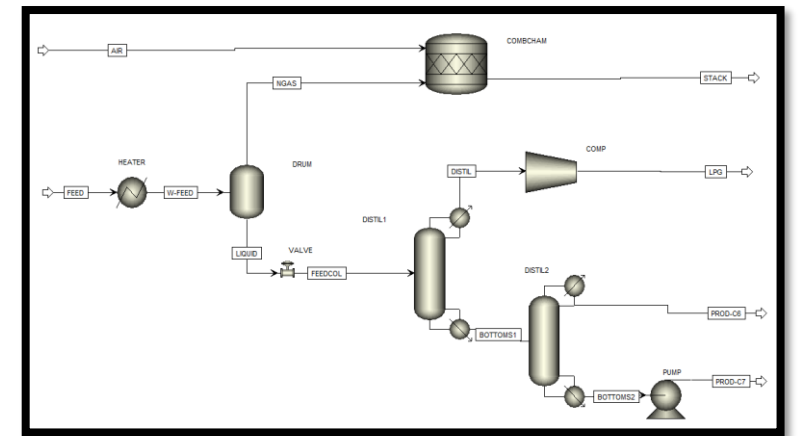
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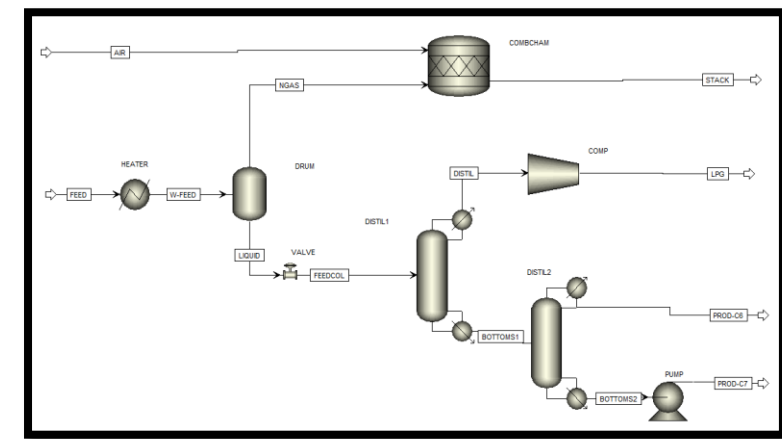
Problem Statement



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 - Recommended operation is partial vapor in order to avoid an extra stage. Reflux
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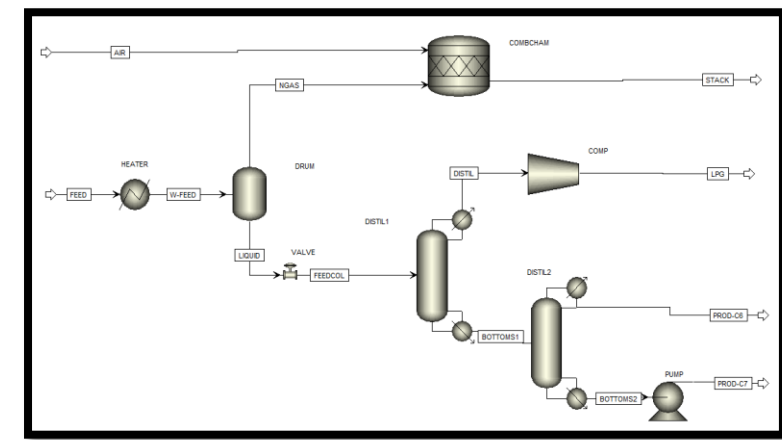
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Problem Statement



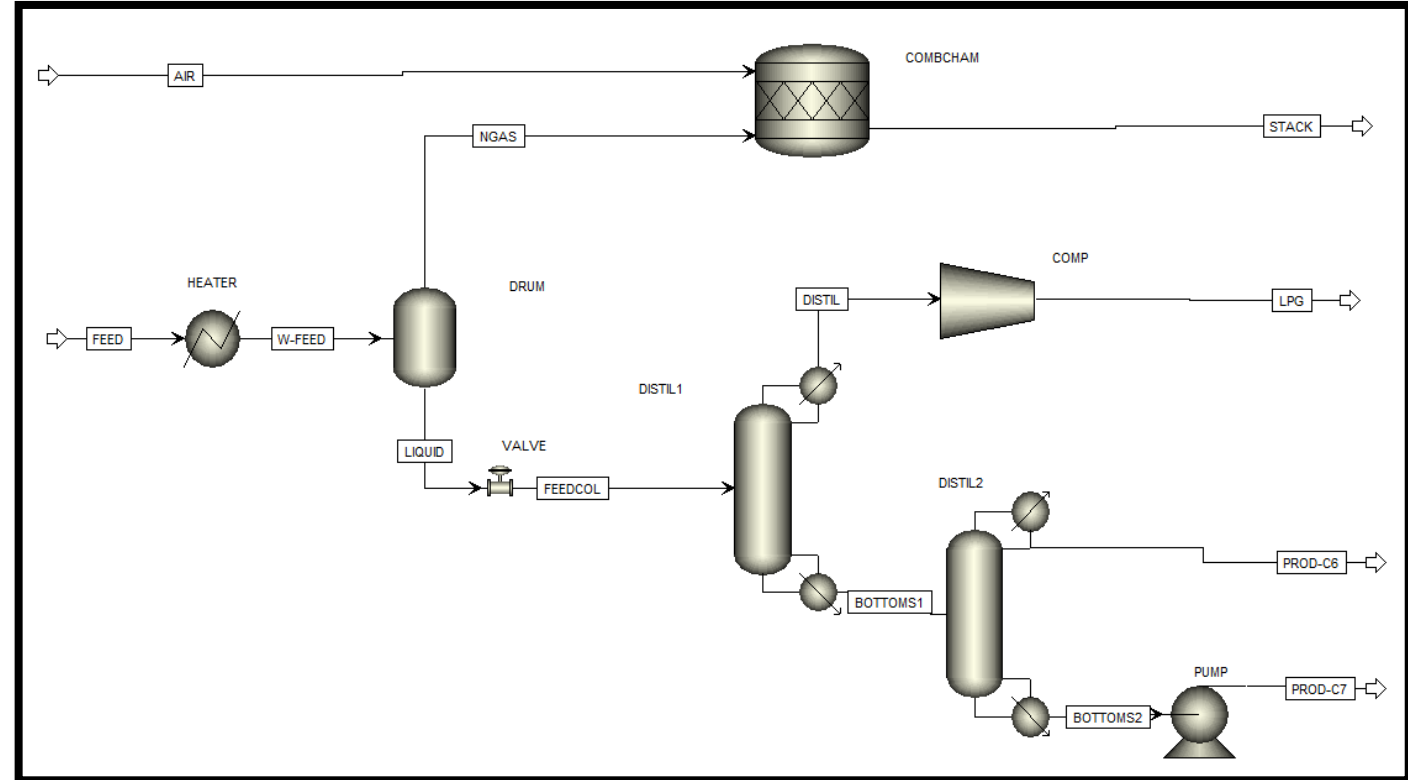
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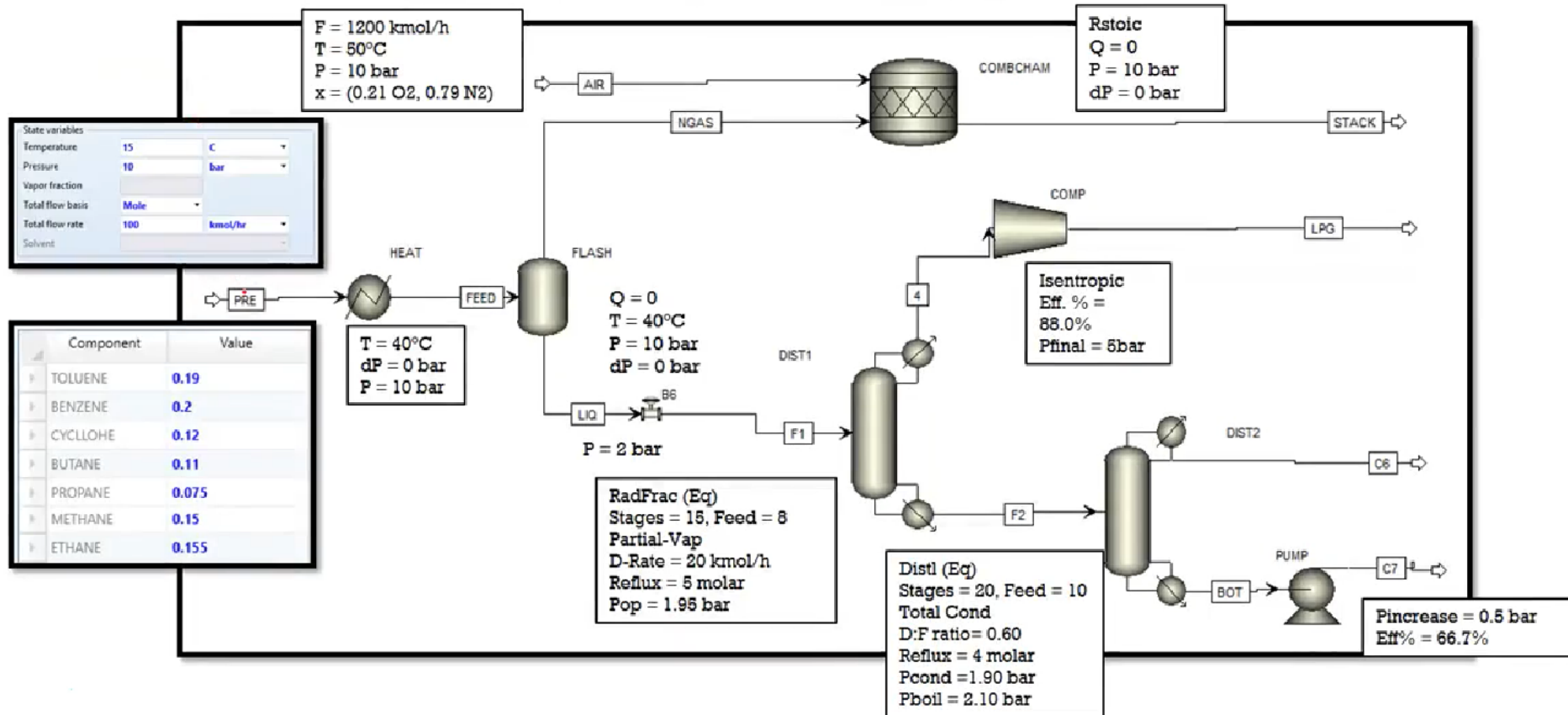
Conditions

- **Unit Operations**

- Heat Exchange
 - Heat Exchanger
- Reaction Kinetics
 - Combustion Chamber / Reactor
- Momentum
 - Pump
 - Compressor
- Separation Process
 - Flash Drum
 - Distillation Columns



Lets try to build this:



Streams

▪ Feed

- $F = 100 \text{ kmol/h}$
- $T = 15^\circ\text{C}$
- $P = 10 \text{ bar}$
- Comp:
 - Toluene 0.190
 - Benzene 0.200
 - Cyclohex 0.120
 - Butane 0.110
 - Propane 0.075
 - Methane 0.150
 - Ethane 0.155

▪ Air

- $F = 1200 \text{ kmol/h}$
- $T = 50^\circ\text{C}$
- $P = 10 \text{ bar}$
- Comp:
 - 0.79 N_2
 - 0.21 O_2

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 50 C

Pressure: 10 bar

Vapor fraction: []

Total flow basis: Mole

Total flow rate: 1200 kmol/hr

Solvent: []

Reference Temperature

Volume flow reference temperature: [] C

Component concentration reference temperature: [] C

Composition

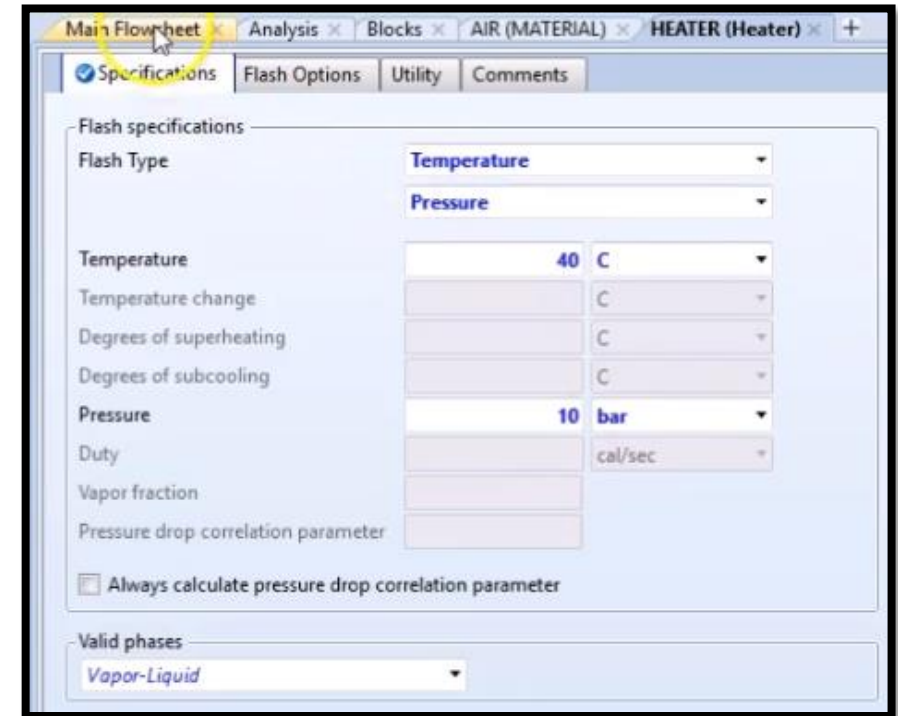
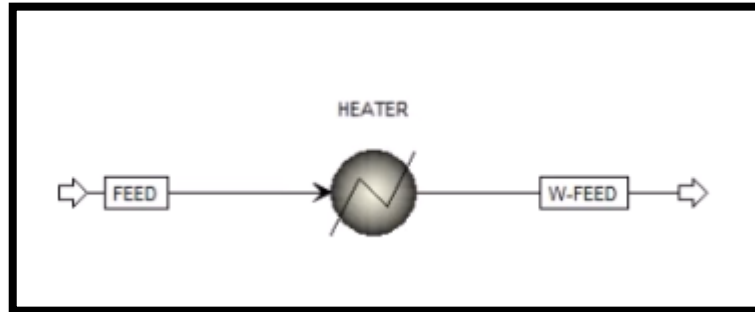
Mole-Flow: kmol/hr

Component	Value
METHANE	
C2	
PROPA-01	
N-BUTANE	
CYCLOHEX	
BENZENE	
TOLUENE	
O2	0.21
N2	0.79
Total	1



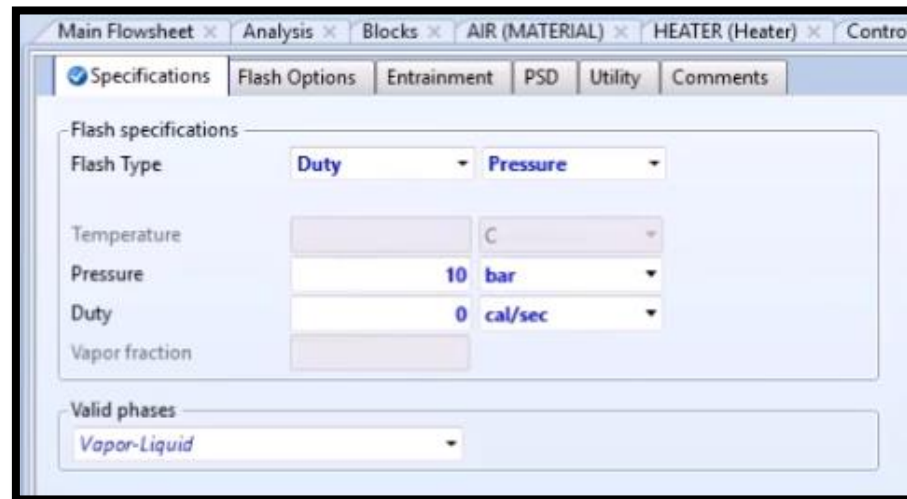
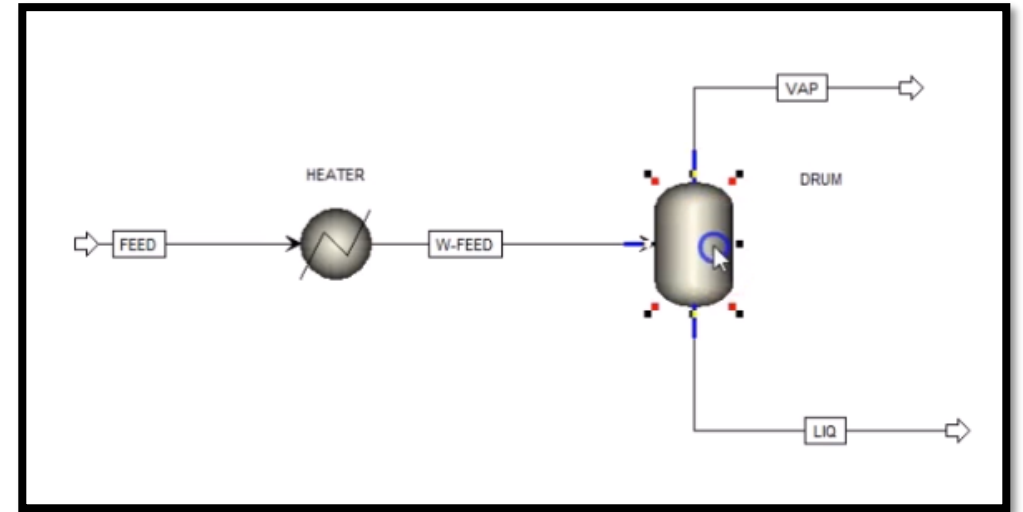
Blocks - Heat Exchanger

- Heater
 - $T = 40^{\circ}\text{C}$
 - $dP = 0 \text{ bar}$
 - $P = 10 \text{ bar}$



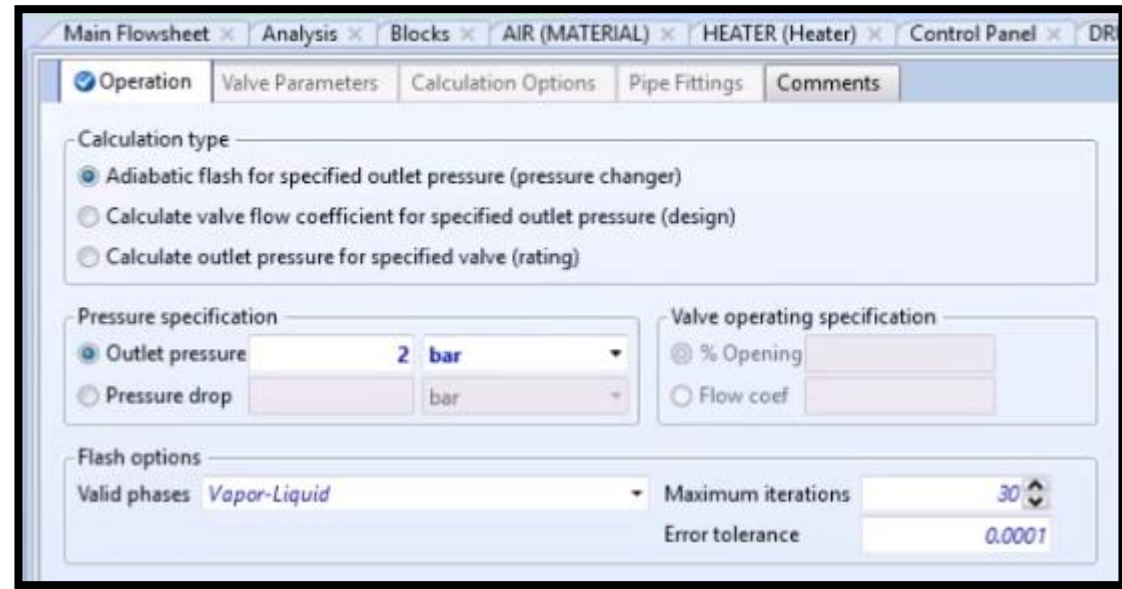
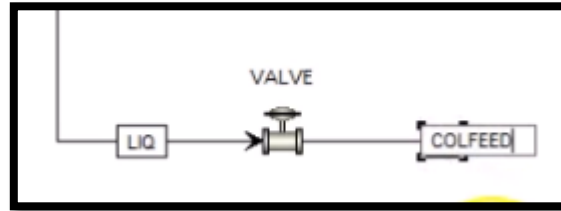
Blocks – Flash Drum

- Flash2
 - $Q = 0$
 - $T = 40^{\circ}\text{C}$
 - $P = 10 \text{ bar}$
 - $dP = 0 \text{ bar}$



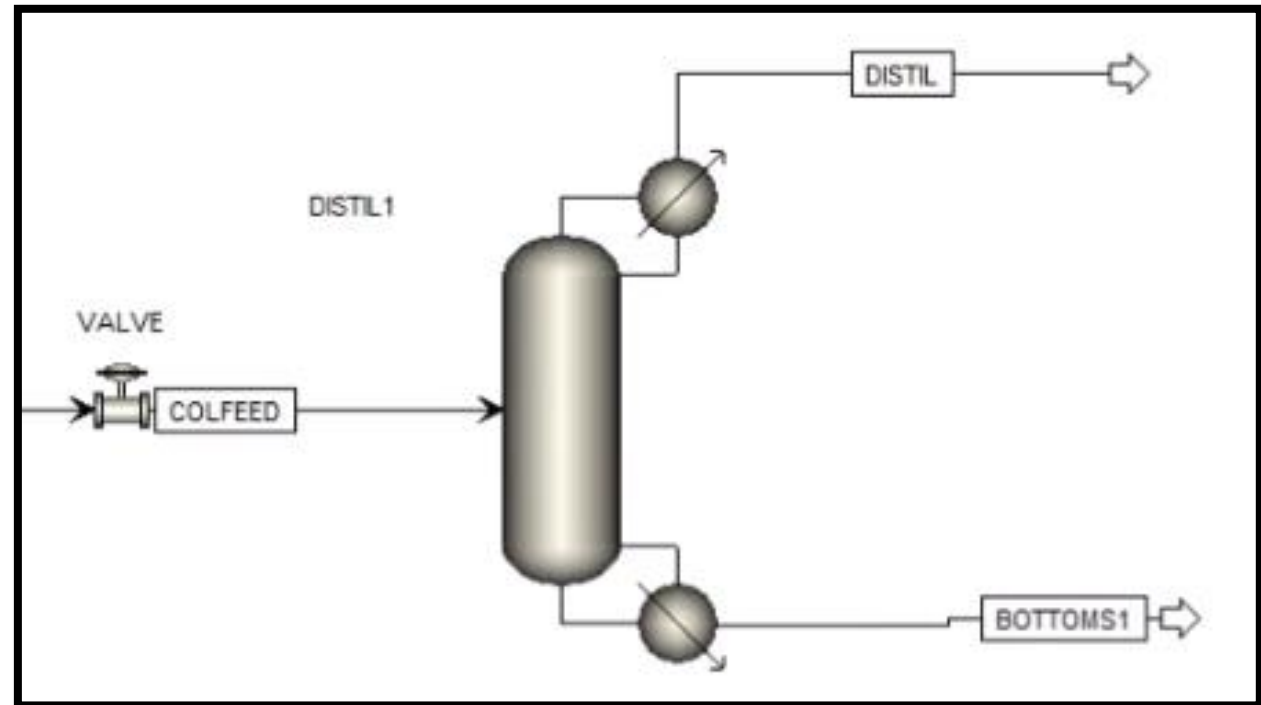
Blocks - Valve

- Valve
 - P = 2 bar



Blocks – Distillation Column 1

- RadFrac
 - Stages = 15
 - Feed = 8
 - Cond = Partial
 - D-Rate = 20 kmol/h
 - Reflux = 5 molar
 - P-reboiler = 1.95 bar



Blocks – Distillation Column 1

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 - Feed = 8
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 - D-Rate = 20 kmol/h
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 - P-reboiler = 1.95 bar

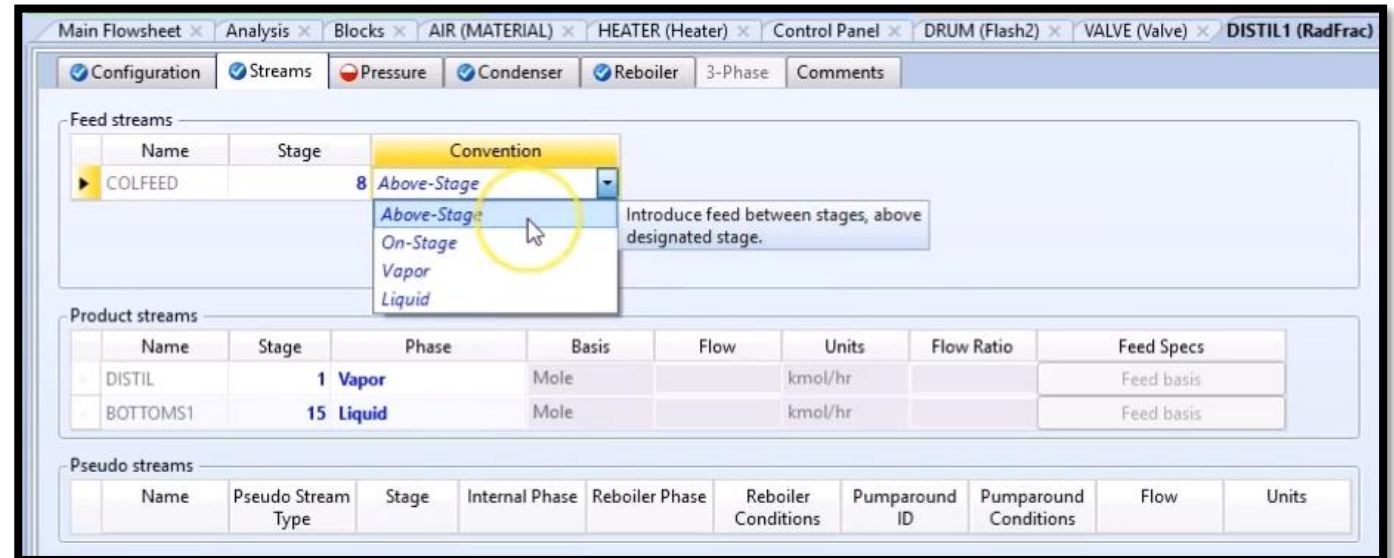
The screenshot shows the configuration window for a RadFrac distillation column. The window has several tabs at the top: Main Flowsheet, Analysis, Blocks, AIR (MATERIAL), HEATER (Heater), Control Panel, and DRUM (Flash2). The 'Configuration' tab is active. Below the tabs, there are several sections:

- Setup options:**
 - Calculation type: Equilibrium
 - Number of stages: 15 (with a 'Stage Wizard' button)
 - Condenser: Partial-Vapor
 - Reboiler: Kettle
 - Valid phases: Vapor-Liquid
 - Convergence: Standard
- Operating specifications:**
 - Distillate rate: 20 kmol/hr (Mole basis)
 - Reflux ratio: 5 (Mole basis)
 - Free water reflux ratio: 0 (Feed Basis)
- A button at the bottom: Design and specify column internals



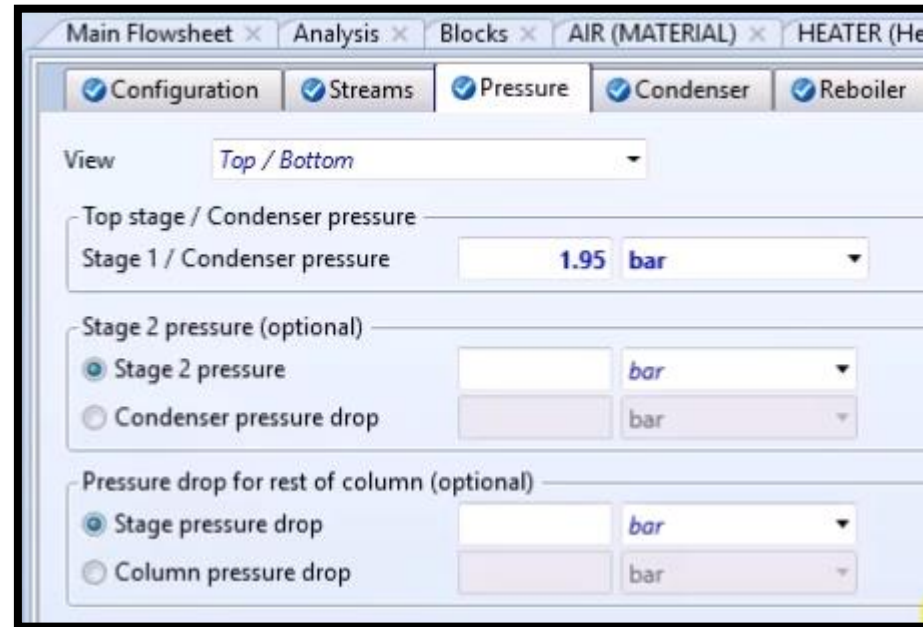
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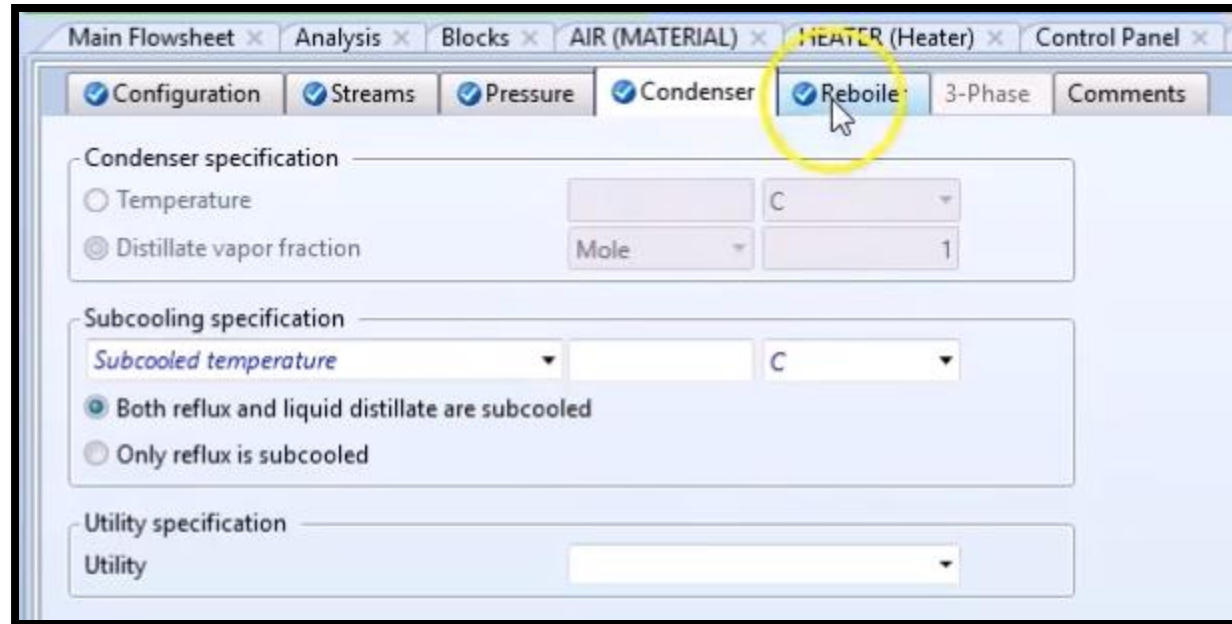
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Blocks – Distillation Column 1

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 - Stages = 15
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 - Cond = Partial
 - D-Rate = 20 kmol/h
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Main Flowsheet x Analysis x Blocks x AIR (MATERIAL) x HEATER (Heater) x Control Panel x D

Configuration Streams Pressure Condenser Reboiler 3-Phase Comments

Thermosiphon reboiler options

- Specify reboiler flow rate
- Specify reboiler outlet condition
- Specify both flow and outlet condition

Reboiler Wizard

Flow rate: Mole kmol/hr

Outlet condition: Temperature C

Optional

Reboiler pressure: bar

Reboiler return feed convention: Above-Stage

Utility:

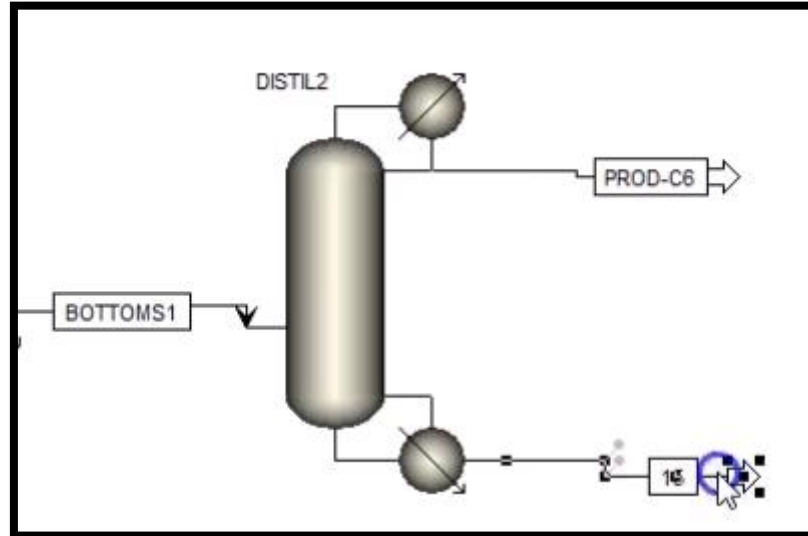
Reboiler configurations

- Circulation without baffle
- Circulation with baffle
- Circulation with auxiliary baffle (Need enough liquid return)



Blocks – Distillation Column 2

- Distil
 - Stages = 20
 - Feed = 10
 - Cond = Total
 - D:F Ratio = 0.60
 - Reflux = 4 molar
 - P-cond = 1.90 bar
 - P-reboiler = 2.10 bar

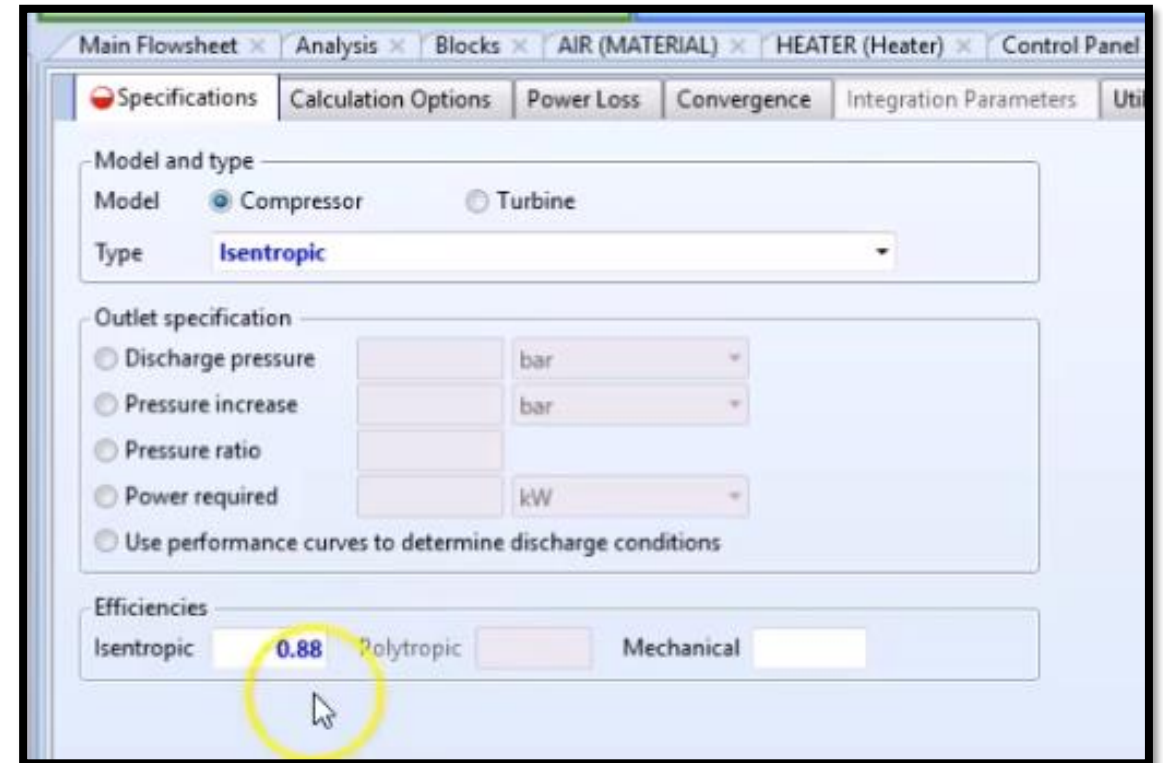
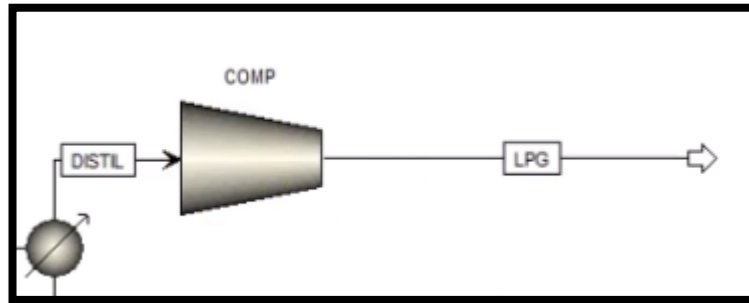


Main Flowsheet × Analysis × Blocks × AIR (MATERIAL) × HEATER (Heater) × Contr	
Specifications	
Convergence	
Comments	
Column specifications	
Number of stages	20
Feed stage	10
Reflux ratio	4
Distillate to feed mole ratio	0.6
Condenser type	Total
Pressure specifications	
Condenser pressure	1.9 bar
Reboiler pressure	2.1 bar



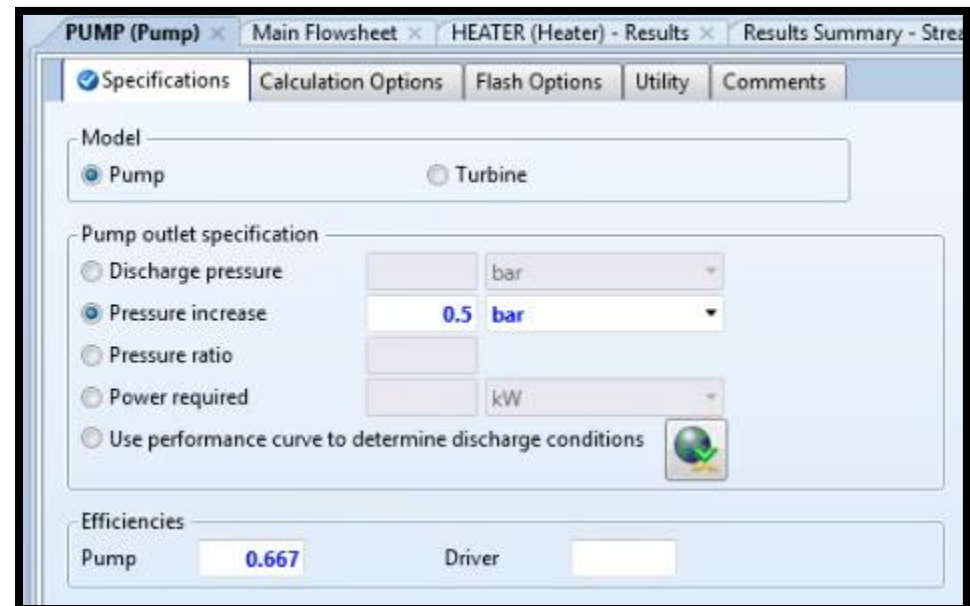
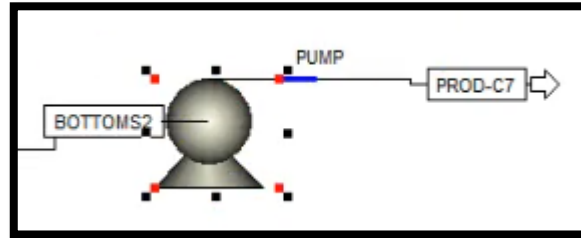
Blocks – Compressor

- Compr
 - Type = Isentropic
 - Eff = 88%
 - P-final = 5 bar



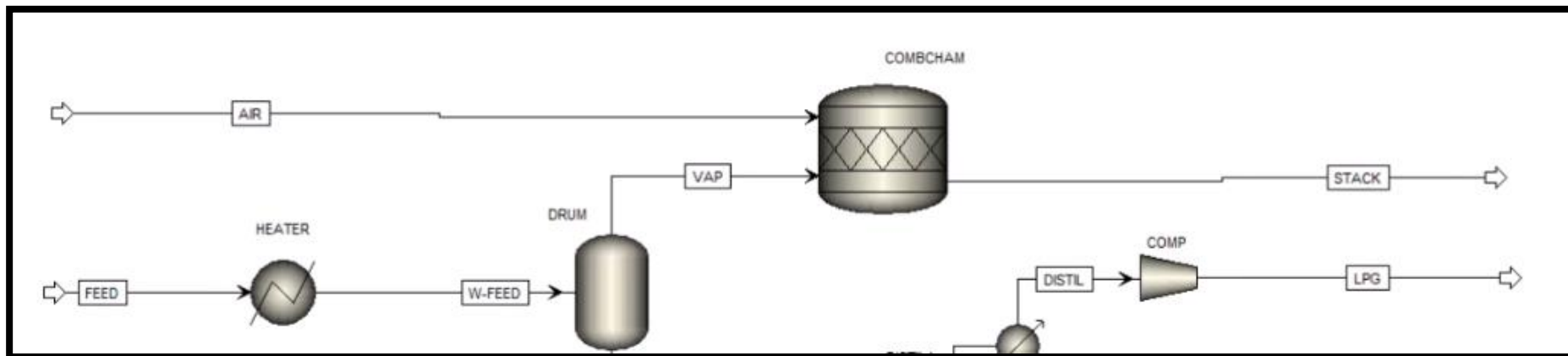
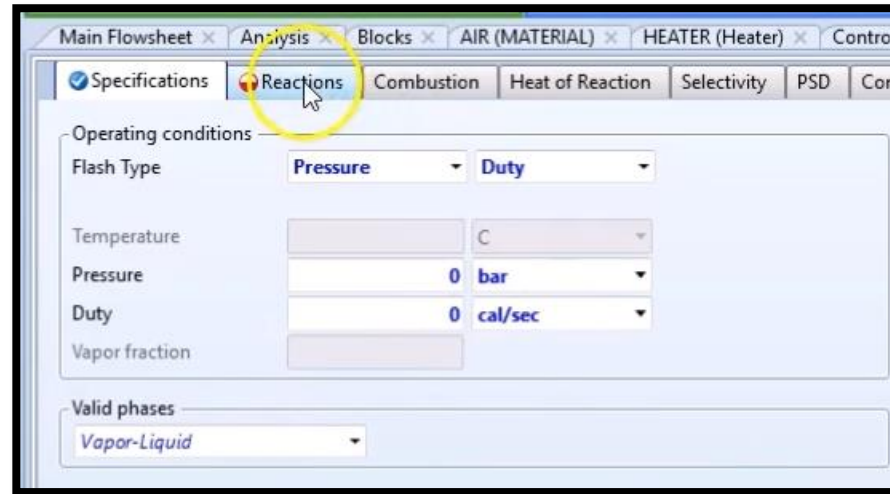
Blocks – Pump

- Pump
 - Type = Isentropic
 - Eff = 66.7%
 - P-increase = 0.5 bar



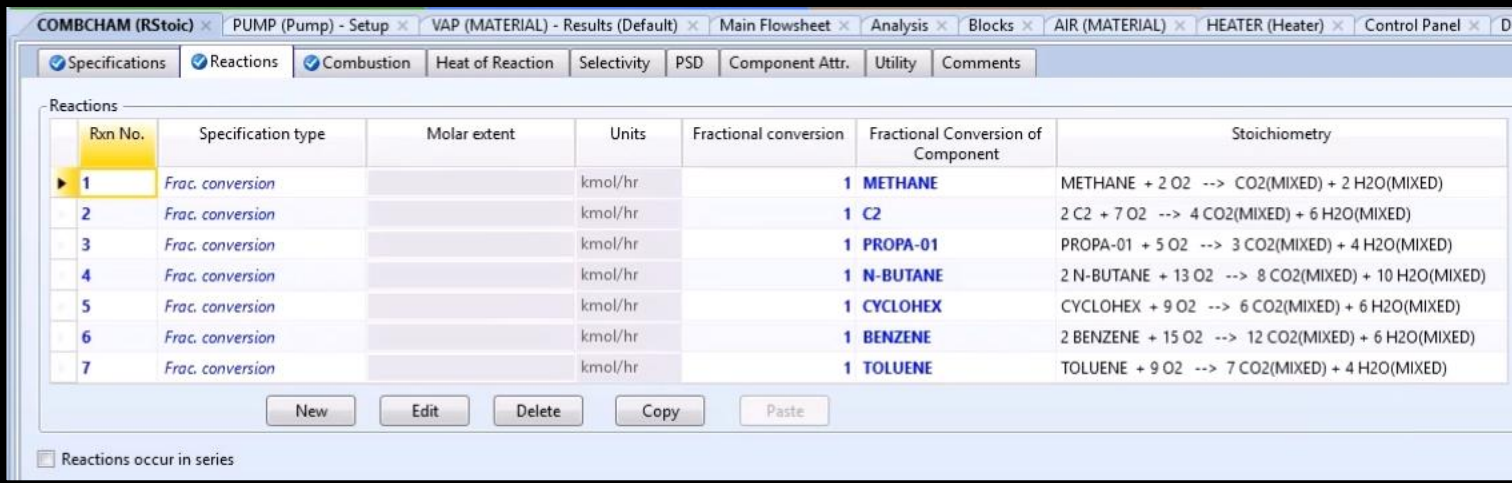
Blocks – Combustion Chamber

- RSTOIC
 - Type = Stoichiometry
 - $Q = 0$
 - $P = 10 \text{ bar}$
 - $dP = 0 \text{ bar}$



Blocks – Combustion Chamber

- RXN
 - $\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O}$
 - $\text{C}_2\text{H}_6 + 7\text{O}_2 = 4\text{CO}_2 + 6\text{H}_2\text{O}$
 - $\text{C}_3\text{H}_8 + 5\text{O}_2 = 3\text{CO}_2 + 4\text{H}_2\text{O}$
 - $2\text{C}_4\text{H}_{10} + 13\text{O}_2 = 8\text{CO}_2 + 10\text{H}_2\text{O}$
 - $\text{C}_6\text{H}_{12} + 6\text{O}_2 = 3\text{CO}_2 + 6\text{H}_2\text{O}$
 - $2\text{C}_6\text{H}_6 + 15\text{O}_2 = 12\text{CO}_2 + 6\text{H}_2\text{O}$
 - $\text{C}_7\text{H}_8 + 9\text{O}_2 = 7\text{CO}_2 + 4\text{H}_2\text{O}$



The screenshot shows the 'Reactions' tab in the COMBCHAM (RStoic) software. The table lists seven reactions, each with a reaction number, specification type, molar extent, units, fractional conversion, fractional conversion of component, and stoichiometry.

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion		kmol/hr		1 METHANE	METHANE + 2 O2 --> CO2(MIXED) + 2 H2O(MIXED)
2	Frac. conversion		kmol/hr		1 C2	2 C2 + 7 O2 --> 4 CO2(MIXED) + 6 H2O(MIXED)
3	Frac. conversion		kmol/hr		1 PROPANE-01	PROPANE-01 + 5 O2 --> 3 CO2(MIXED) + 4 H2O(MIXED)
4	Frac. conversion		kmol/hr		1 N-BUTANE	2 N-BUTANE + 13 O2 --> 8 CO2(MIXED) + 10 H2O(MIXED)
5	Frac. conversion		kmol/hr		1 CYCLOHEX	CYCLOHEX + 9 O2 --> 6 CO2(MIXED) + 6 H2O(MIXED)
6	Frac. conversion		kmol/hr		1 BENZENE	2 BENZENE + 15 O2 --> 12 CO2(MIXED) + 6 H2O(MIXED)
7	Frac. conversion		kmol/hr		1 TOLUENE	TOLUENE + 9 O2 --> 7 CO2(MIXED) + 4 H2O(MIXED)

Buttons: New, Edit, Delete, Copy, Paste

Reactions occur in series



Save File!



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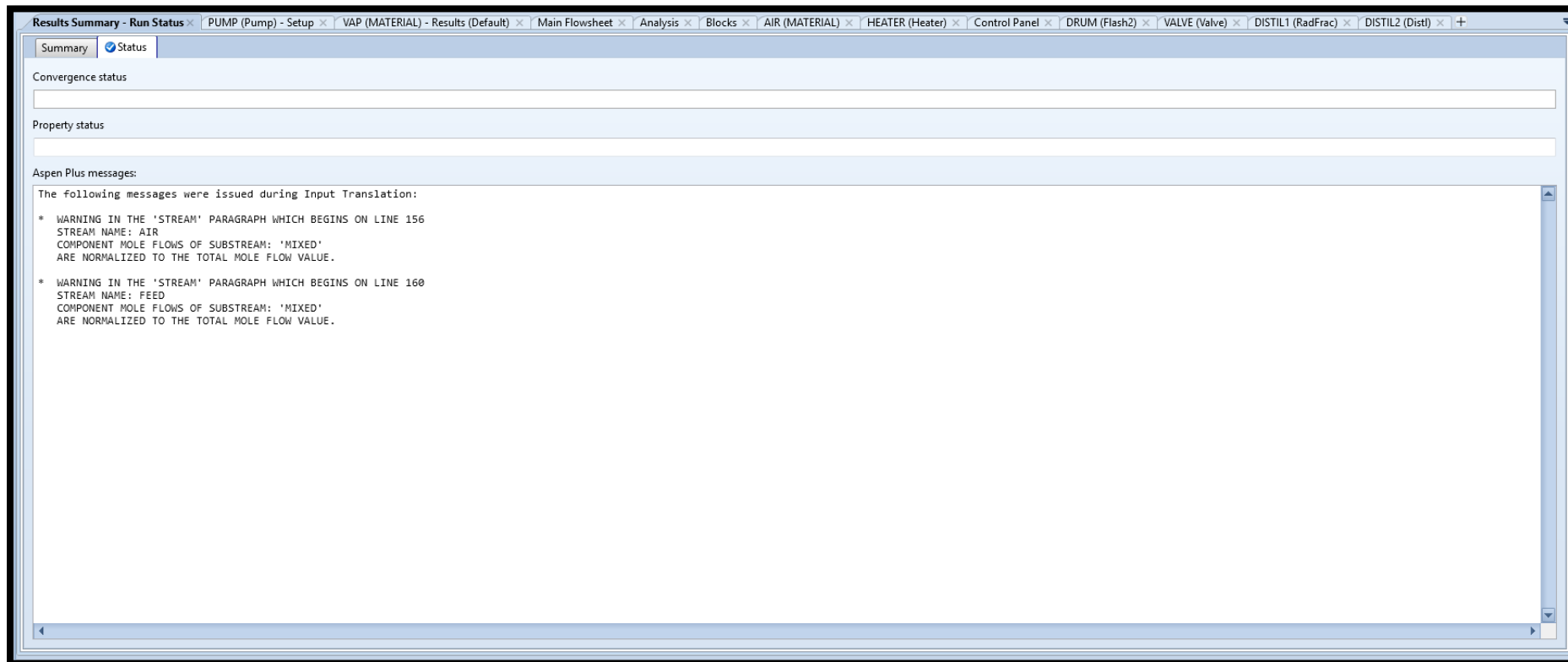
Running, Results & Analysis

- Running the simulation
 - Errors & Debugging
- Getting Results
 - Stream Results
 - Block Results
- Analysis
 - What if Scenarios



Running the Simulation

- Error Messages



Getting Stream Results

Results Summary - Streams (All) | DISTIL1 (RadFrac) - Results | PROD-C6 (MATERIAL) - Results (Default) | Results Summary - Run Status | PUMP (Pump) - Setup | VAP (MATERIAL) - Results (Default) | Main Flowsheet | Analysis | Blocks | AIR (MATERIAL) | TER (Heater) | +

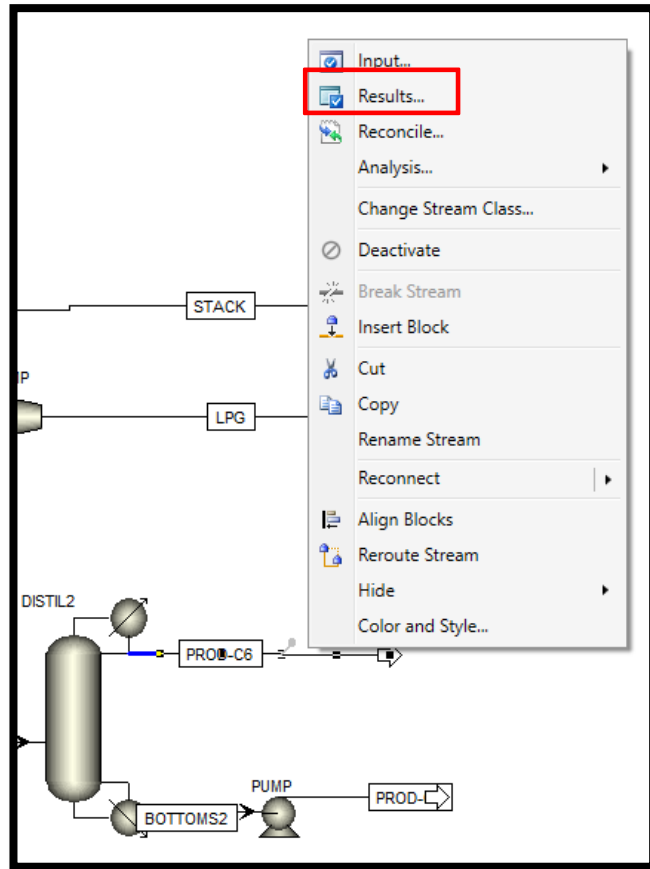
Material | Heat | Load | Work | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

Sum: 10153.5

Material	Units	BOTTOMS1	BOTTOMS2	COLFEED	DISTIL	FEED	LIQ	LPG	PROD-C6	PROD-C7	STACK	VAP	W-FEED
Molar Density	mol/cc	0.00887379	0.00816443	0.000651575	8.15994e-05	0.0015948	0.0101947	0.000193645	0.00934497	0.00816398	9.22889e-05	0.000408329	0.00122446
Mass Density	gm/cc	0.753306	0.74826	0.0483167	0.00388533	0.0956828	0.755973	0.00922034	0.751204	0.748219	0.00263436	0.0113674	0.0734636
Enthalpy Flow	cal/sec	4918.25	37762.7	-188442	-135027	-378537	-188442	-131514	-30424	37774.7	-113942	-166711	-355152
Average MW		84.8911	91.6487	74.1537	47.6147	59.9968	74.1537	47.6147	80.3859	91.6487	28.5447	27.8388	59.9968
+ Mole Flows	kmol/hr	49.4333	19.7733	69.4333	20	100	69.4333	20	29.66	19.7733	1242.66	30.5667	100
- Mole Fractions													
METHANE		7.64126e-22	0	0.0142686	0.0495358	0.15	0.0142686	0.0495358	0	0	0	0.458318	0.15
C2		6.79459e-16	0	0.0662011	0.229828	0.155	0.0662011	0.229828	0	0	0	0.35671	0.155
PROPA-01		2.01073e-12	0	0.062759	0.217878	0.075	0.062759	0.217278	3.35121e-12	0	0	0.102806	0.075
N-BUTANE		1.24588e-08	0	0.130493	0.453029	0.11	0.130493	0.453021	2.07647e-08	0	0	0.063449	0.11
CYCLOHEX		0.233528	0.0234228	0.170325	0.0141078	0.12	0.170325	0.0141078	0.373598	0.0234228	0	0.00568554	0.12
BENZENE		0.383983	0.0217369	0.283637	0.0356162	0.2	0.283637	0.0356162	0.625481	0.0217369	0	0.0100147	0.2
TOLUENE		0.382489	0.95484	0.272316	5.45676e-06	0.19	0.272316	5.45676e-06	0.000921004	0.95484	0	0.00301676	0.19
O2		0	0	0	0	0	0	0	0	0	0.122971	0	0
N2		0	0	0	0	0	0	0	0	0	0.762878	0	0
CO2		0	0	0	0	0	0	0	0	0	0.0454879	0	0
H2O		0	0	0	0	0	0	0	0	0	0.0686636	0	0
+ Mass Flows	kg/hr	4196.44	1812.2	5148.74	952.294	5999.68	5148.74	952.294	2384.25	1812.2	35471.4	850.941	5999.68
+ Mass Fractions													
Volume Flow	l/min	92.8451	40.3647	1776.04	4085	1045.06	113.512	1721.36	52.8983	40.367	224415	1247.63	1361.15
+ Vapor Phase													
+ Liquid Phase													
<add properties>													



Getting Stream Results

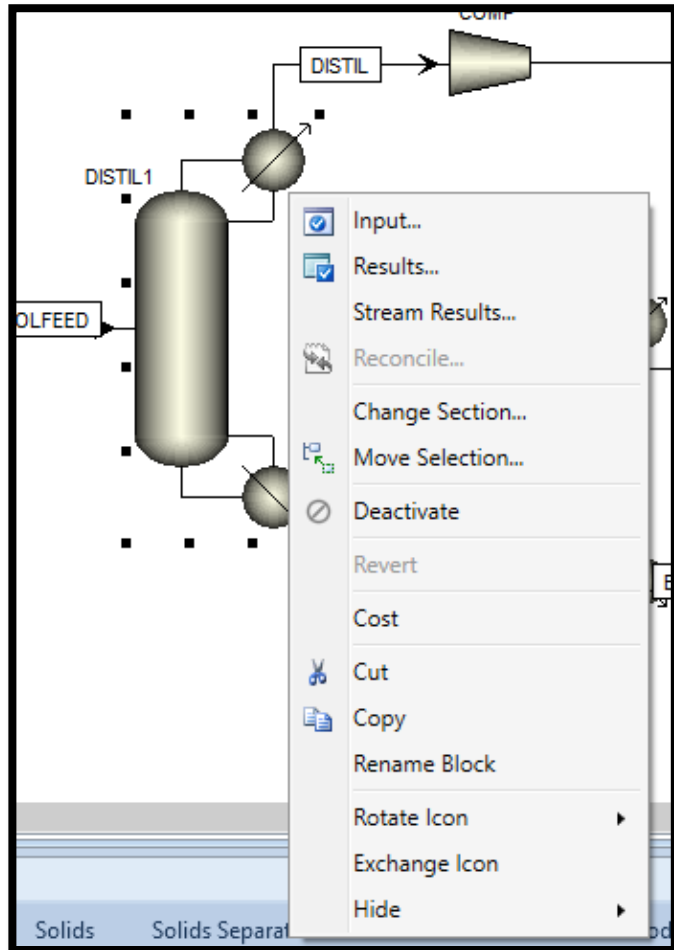


	Units	PROD-C6
MIXED Substream		
Phase		Liquid Phase
Temperature	C	102.643
Pressure	bar	1.9
Molar Vapor Fraction		0
Molar Liquid Fraction		1
Molar Solid Fraction		0
Mass Vapor Fraction		0
Mass Liquid Fraction		1
Mass Solid Fraction		0
Molar Enthalpy	cal/mol	-3692.74
Mass Enthalpy	cal/gm	-45.9376
Molar Entropy	cal/mol-K	-82.6706
Mass Entropy	cal/gm-K	-1.02842
Molar Density	mol/cc	0.00934497
Mass Density	gm/cc	0.751204
Enthalpy Flow	cal/sec	-30424
Average MW		80.3859
Mole Flows	kmol/hr	29.66
METHANE	kmol/hr	0
C2	kmol/hr	0
PROPA-01	kmol/hr	9.93969e-11
N-BUTANE	kmol/hr	6.1588e-07
CYCLOHEX	kmol/hr	11.0809

	Units	PROD-C6
Mole Flows	kmol/hr	29.66
METHANE	kmol/hr	0
C2	kmol/hr	0
PROPA-01	kmol/hr	9.93969e-11
N-BUTANE	kmol/hr	6.1588e-07
CYCLOHEX	kmol/hr	11.0809
BENZENE	kmol/hr	18.5517
TOLUENE	kmol/hr	0.0273169
O2	kmol/hr	0
N2	kmol/hr	0
CO2	kmol/hr	0
H2O	kmol/hr	0
Mole Fractions		
METHANE		0
C2		0
PROPA-01		3.35121e-12
N-BUTANE		2.07647e-08
CYCLOHEX		0.373598
BENZENE		0.625481
TOLUENE		0.000921004
O2		0
N2		0
CO2		0
H2O		0



Getting Block Results



DISTIL1 (RadFrac) - Results x PROD-C6 (MATERIAL) - Results (Default) x Results Summary -

Summary Balance Split Fraction Reboiler Utilities Stage Utilities Status

Basis: Mole

Condenser / Top stage performance

Name	Value	Units
Temperature	25.3431	C
Subcooled temperature		
Heat duty	-227468	cal/sec
Subcooled duty		
Distillate rate	20	kmol/hr
Reflux rate	100	kmol/hr
Reflux ratio	5	
Free water distillate rate		
Free water reflux ratio		

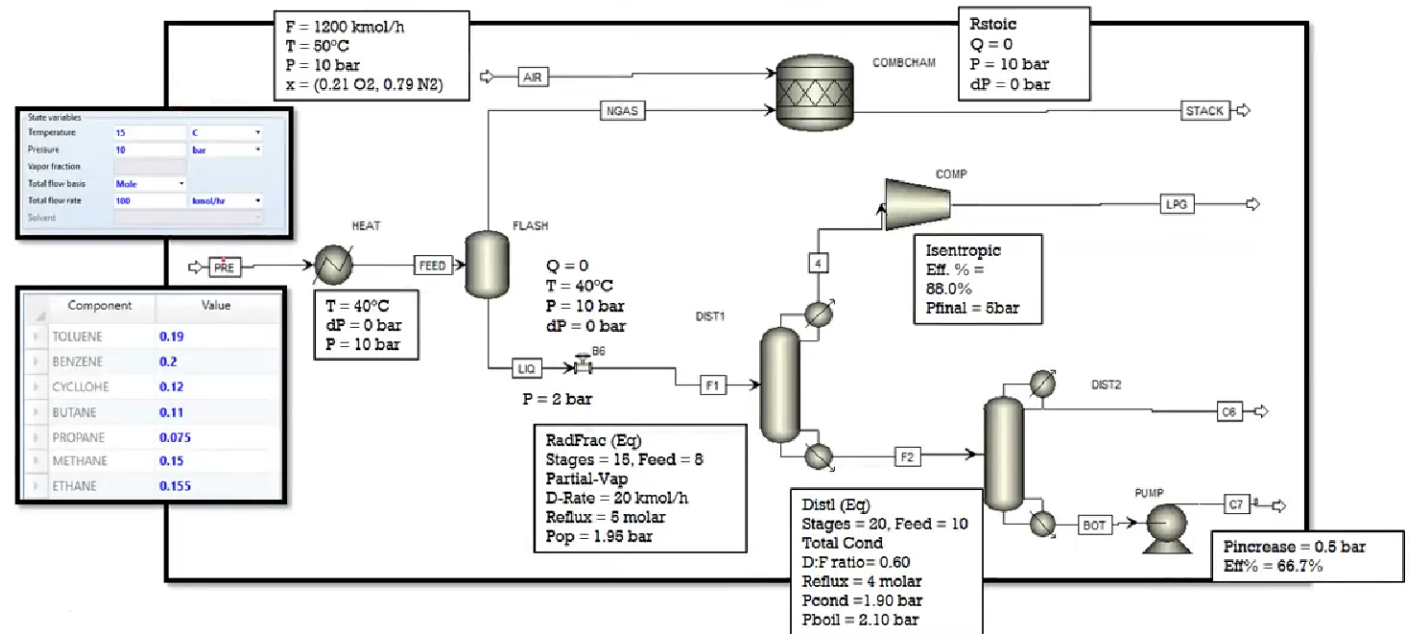
Reboiler / Bottom stage performance

Name	Value	Units
Temperature	113.747	C
Heat duty	285802	cal/sec
Bottoms rate	49.4333	kmol/hr
Boilup rate	142.104	kmol/hr
Boilup ratio	2.87466	
Bottoms to feed ratio		



Analysis

- Manual “what if” cases
 - Change several inputs to get new outputs
 - Change of T Heat
 - Change of P valve
 - Change of P Reactor
 - Changer of Reflux Dist1
 - Change of Stages Dist2



My results

- Compare your results with mine:

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1242.66	20	29.66	19.7733
METHANE	kmol/hr	0	0.990716	0	0
C2	kmol/hr	0	4.59656	0	0
PROPA-01	kmol/hr	0	4.35757	9.93969e-11	0
N-BUTANE	kmol/hr	0	9.06057	6.1588e-07	0
CYCLOHEX	kmol/hr	0	0.282155	11.0809	0.463146
BENZENE	kmol/hr	0	0.712325	18.5517	0.42981
TOLUENE	kmol/hr	0	0.000109135	0.0273169	18.8804
O2	kmol/hr	152.811	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	56.5261	0	0	0
H2O	kmol/hr	85.3257	0	0	0
- Mole Fractions					
METHANE		0	0.0495358	0	0
C2		0	0.229828	0	0
PROPA-01		0	0.217878	3.35121e-12	0
N-BUTANE		0	0.453029	2.07647e-08	0
CYCLOHEX		0	0.0141078	0.373598	0.0234228
BENZENE		0	0.0356162	0.625481	0.0217369
TOLUENE		0	5.45676e-06	0.000921004	0.95484
O2		0.122971	0	0	0
N2		0.762878	0	0	0
CO2		0.0454879	0	0	0
H2O		0.0686636	0	0	0



CASE A - Change of T Heat

- Change $T = 40^{\circ}\text{C}$ to $T = 30^{\circ}\text{C}$ of Heater

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1242.66	20	29.66	19.7733
METHANE	kmol/hr	0	0.990716	0	0
C2	kmol/hr	0	4.59656	0	0
PROPA-01	kmol/hr	0	4.35757	9.93969e-11	0
N-BUTANE	kmol/hr	0	9.06057	6.1588e-07	0
CYCLOHEX	kmol/hr	0	0.282155	11.0809	0.463146
BENZENE	kmol/hr	0	0.712325	18.5517	0.42981
TOLUENE	kmol/hr	0	0.000109135	0.0273169	18.8804
O2	kmol/hr	152.811	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	56.5261	0	0	0
H2O	kmol/hr	85.3257	0	0	0
- Mole Fractions					
METHANE		0	0.0495358	0	0
C2		0	0.229828	0	0
PROPA-01		0	0.217878	3.35121e-12	0
N-BUTANE		0	0.453029	2.07647e-08	0
CYCLOHEX		0	0.0141078	0.373598	0.0234228
BENZENE		0	0.0356162	0.625481	0.0217369
TOLUENE		0	5.45676e-06	0.000921004	0.95484
O2		0.122971	0	0	0
N2		0.762878	0	0	0
CO2		0.0454879	0	0	0
H2O		0.0686636	0	0	0

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1238.26	20	31.0797	20.7198
METHANE	kmol/hr	0	1.15624	0	0
C2	kmol/hr	0	5.47187	1.00933e-10	0
PROPA-01	kmol/hr	0	4.92073	3.38701e-06	0
N-BUTANE	kmol/hr	0	8.45116	1.1446	5.72647e-12
CYCLOHEX	kmol/hr	0	3.8388e-10	10.985	0.909186
BENZENE	kmol/hr	0	3.52203e-09	18.9357	0.877564
TOLUENE	kmol/hr	0	5.43581e-14	0.0144238	18.933
O2	kmol/hr	164.364	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	49.3783	0	0	0
H2O	kmol/hr	76.5157	0	0	0
- Mole Fractions					
METHANE		0	0.0578118	0	0
C2		0	0.273593	3.24757e-12	0
PROPA-01		0	0.246037	1.08978e-07	0
N-BUTANE		0	0.422558	0.0368278	2.76377e-13
CYCLOHEX		0	1.9194e-11	0.353447	0.0438801
BENZENE		0	1.76102e-10	0.609262	0.0423539
TOLUENE		0	2.71791e-15	0.000464093	0.913765
O2		0.132738	0	0	0
N2		0.765592	0	0	0
CO2		0.0398773	0	0	0
H2O		0.061793	0	0	0



CASE B - Change of P valve

- Change Pressure of Valve
 - P = 1 bar
 - P = 5 bar

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1242.66	20	29.66	19.7733
METHANE	kmol/hr	0	0.990716	0	0
C2	kmol/hr	0	4.59656	0	0
PROPA-01	kmol/hr	0	4.35757	9.93969e-11	0
N-BUTANE	kmol/hr	0	9.06057	6.1588e-07	0
CYCLOHEX	kmol/hr	0	0.282155	11.0809	0.463146
BENZENE	kmol/hr	0	0.712325	18.5517	0.42981
TOLUENE	kmol/hr	0	0.000109135	0.0273169	18.8804
O2	kmol/hr	152.811	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	56.5261	0	0	0
H2O	kmol/hr	85.3257	0	0	0
- Mole Fractions					
METHANE		0	0.0495358	0	0
C2		0	0.229828	0	0
PROPA-01		0	0.217878	3.35121e-12	0
N-BUTANE		0	0.453029	2.07647e-08	0
CYCLOHEX		0	0.0141078	0.373598	0.0234228
BENZENE		0	0.0356162	0.625481	0.0217369
TOLUENE		0	5.45676e-06	0.000921004	0.95484
O2		0.122971	0	0	0
N2		0.762878	0	0	0
CO2		0.0454879	0	0	0
H2O		0.0686636	0	0	0

No Drastic Change



CASE C - Change of P Reactor

- Change Pressure of Reactor
 - P = -5bar
 - P = 1bar

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1242.66	20	29.66	19.7733
METHANE	kmol/hr	0	0.990716	0	0
C2	kmol/hr	0	4.59656	0	0
PROPA-01	kmol/hr	0	4.35757	9.93969e-11	0
N-BUTANE	kmol/hr	0	9.06057	6.1588e-07	0
CYCLOHEX	kmol/hr	0	0.282155	11.0809	0.463146
BENZENE	kmol/hr	0	0.712325	18.5517	0.42981
TOLUENE	kmol/hr	0	0.000109135	0.0273169	18.8804
O2	kmol/hr	152.811	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	56.5261	0	0	0
H2O	kmol/hr	85.3257	0	0	0
- Mole Fractions					
METHANE		0	0.0495358	0	0
C2		0	0.229828	0	0
PROPA-01		0	0.217878	3.35121e-12	0
N-BUTANE		0	0.453029	2.07647e-08	0
CYCLOHEX		0	0.0141078	0.373598	0.0234228
BENZENE		0	0.0356162	0.625481	0.0217369
TOLUENE		0	5.45676e-06	0.000921004	0.95484
O2		0.122971	0	0	0
N2		0.762878	0	0	0
CO2		0.0454879	0	0	0
H2O		0.0686636	0	0	0



CASE D - Change of Reflux Dist2

- Change Reflux Ratio from 4 to 2 and/or 6 and/or 15

	Units	STACK	LPG	PROD-C6	PROD-C7
- Mole Flows	kmol/hr	1242.66	20	29.66	19.7733
METHANE	kmol/hr	0	0.990716	0	0
C2	kmol/hr	0	4.59656	0	0
PROPA-01	kmol/hr	0	4.35757	9.93969e-11	0
N-BUTANE	kmol/hr	0	9.06057	6.1588e-07	0
CYCLOHEX	kmol/hr	0	0.282155	11.0809	0.463146
BENZENE	kmol/hr	0	0.712325	18.5517	0.42981
TOLUENE	kmol/hr	0	0.000109135	0.0273169	18.8804
O2	kmol/hr	152.811	0	0	0
N2	kmol/hr	948	0	0	0
CO2	kmol/hr	56.5261	0	0	0
H2O	kmol/hr	85.3257	0	0	0
- Mole Fractions					
METHANE		0	0.0495358	0	0
C2		0	0.229828	0	0
PROPA-01		0	0.217878	3.35121e-12	0
N-BUTANE		0	0.453029	2.07647e-08	0
CYCLOHEX		0	0.0141078	0.373598	0.0234228
BENZENE		0	0.0356162	0.625481	0.0217369
TOLUENE		0	5.45676e-06	0.000921004	0.95484
O2		0.122971	0	0	0
N2		0.762878	0	0	0
CO2		0.0454879	0	0	0
H2O		0.0686636	0	0	0



Course Closure

1. Introduction
2. Our Chemical Process!
3. Setting up the Physical Property Environment
4. Simulation Environment I – The Flowsheet
5. Simulation Environment II – Unit Operations
6. Running, Results & Analysis
7. Case Studies
8. Conclusion



Course Closure

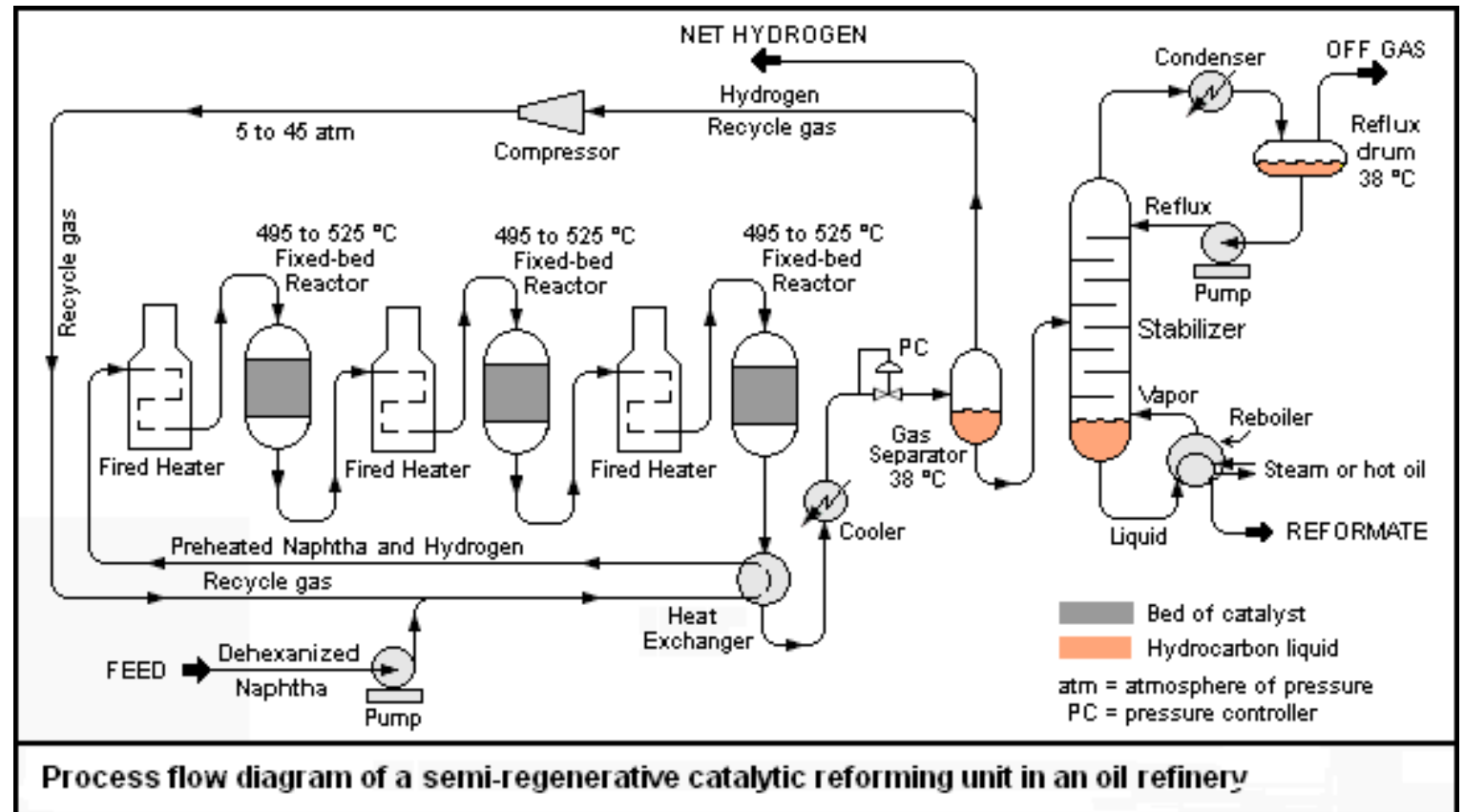
- **Introductory Knowledge of Processes Modeling**
 - General Flowsheet Concepts
 - Setting the adequate Physical Properties
 - Basic Flowsheet “manipulation”
 - Minimum Requirements to set up & run a Simulation
 - Common Unit Operations
 - Create an interest in Process Modeling



Solve this!

Change:

- All T of Reactors
- Feed Composition
- No. of Plates in Distl. Col
- T of Heat Ex
- Gas Sep. T
- Compressor P
- Utility Costs



What's Next?

- Typically, you will follow your training with
 - **Basic Course**
- What do you learn there:
 - More on Aspen Plus
 - More on Physical Property Environment
 - Flowsheet techniques
 - More Unit Operations
 - Analysis Tools
 - Plenty Workshops
 - Process & Industry Case Studies



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