Process Simulation for **Energy Consulting**

Jan. 2018

한국에너지공단
KOREA ENERGY AGENCY

Contents

I. Introduction of Process Simulation

1. General
2. The structure of Process Simulator

1. General

- **The advancement in computer-aided process simulation over the past generation has been nothing short of spectacular. Until the last 1970s, it was rare for a graduating chemical engineer to have any experience in using a chemical process simulator. Most material and energy balances were still done by hand by teams of engineers. The rigorous simulation of multistage separation equipment and complicated reactors was generally unheard of, and the design of such equipment was achieved by combination of simplified analysis, shortcut methods, and years of experience.**
- **In the present day, however, companies of customer now expect ours to be conversant with a wide variety of computer programs, especially a process simulator.**
- **To some extent, the knowledge base required to simulate successfully a chemical process will depend on the simulation used. Currently there are several process simulators on the market, for example, CHEMCAD, INVENSYS(PRO II, Petrosim, etc.), AspenOne(Aspen Plus*, HYSYS**, EDR***, etc.).**
- **KEA has introduced HYSYS from 2000, and developed a lot of solutions for processes using simulator till now. Moreover, KEA has many kinds of simulator since introduced total AspenOne package**** in the first 2012s. KEA's simulators are shown [Table].**

* Aspen Plus : the process simulator based aspen database for chemical process especially petroleum, polymer, etc.

** HYSYS : the process simulator based hysys database for chemical process especially gas, refinery plant, etc.

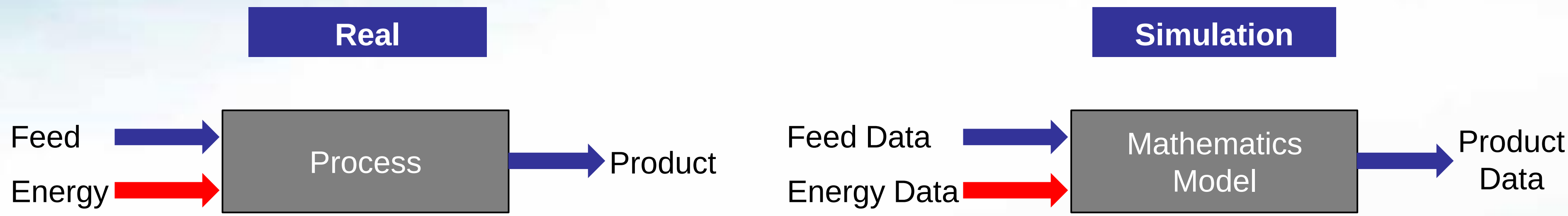
*** EDR : Exchanger Design and Rating simulator consisted of shell&tube, plate, airfin cooler, etc.

**** total Aspenone package is consisted of all aspen simulators. e.g. utility planner, EDR, Aspen Plus, Polymer etc.

Classification	Simulators	Description	Remarks
Process Modeling	Aspen Plus	Petroleum, Chemical Plant	including polymer
	Aspen HYSYS	Refinery, Gas, Chemical Plant	including upstream
	Aspen Flare	Flare analysis	
	Aspen Utility Planner	Utility optimization	
	Aspen Energy Analyzer	Pinch analysis	
	Aspen Properties	Physical properties analysis	For Plus, HYSYS
	Aspen HYSYS Thermodynamic	Physical properties analysis	For HYSYS
	Aspen Reaction Modeler	Custom Reactor Modeling	
Design and Rating	Aspen EDR	Exchanger Design and Rating	Shell&Tube, Plate, Fired heater Plate Fin, etc
Economic evaluation	Aspen Capital Cost, In-plant, Process economy evaluation	Business Feasibility Estimation	

● **What is a process simulation?**

- Process simulation is a activity describing a real process in the plant using computer software.

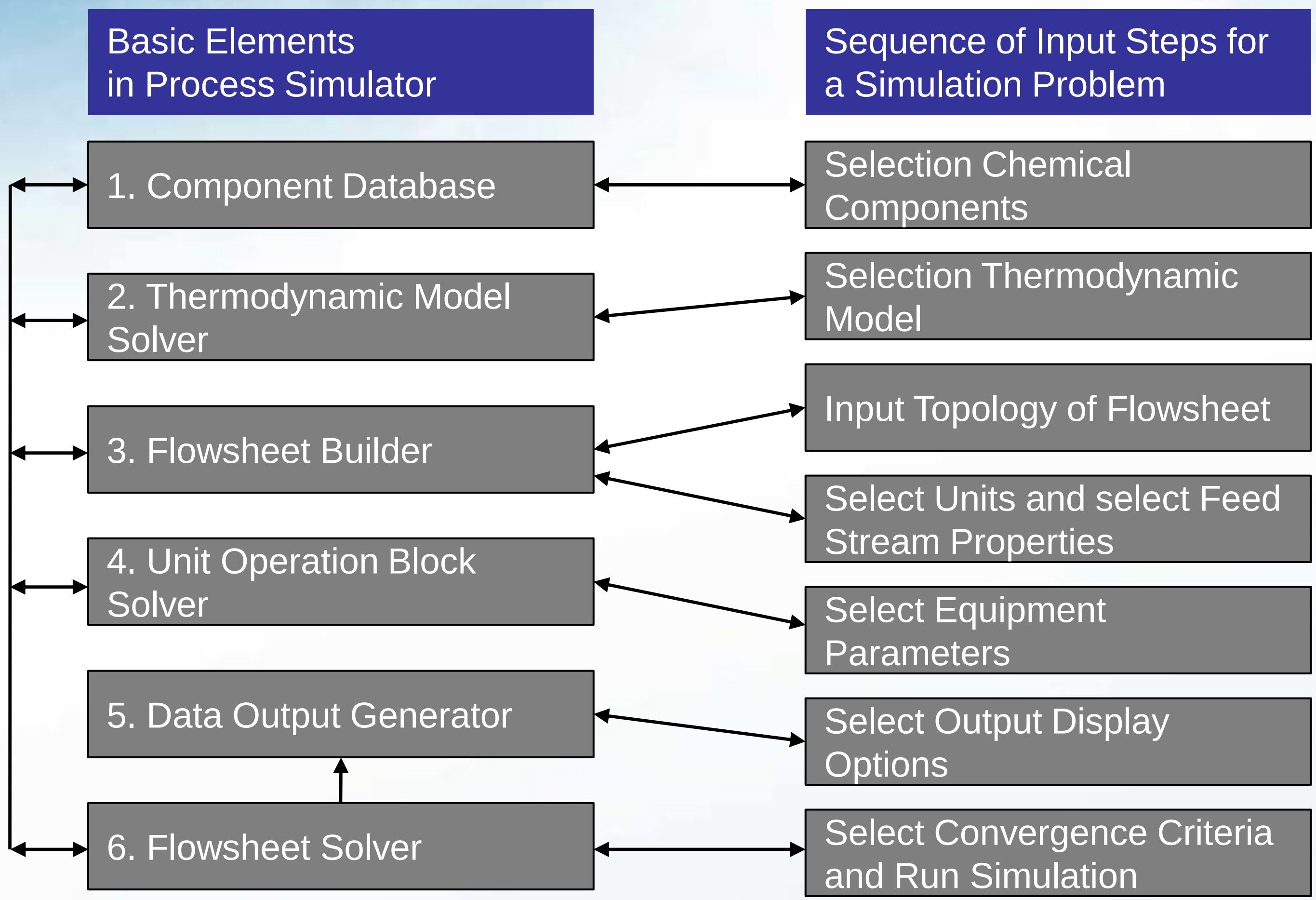


● **Why is a process simulation?**

- Simulation using computer software is mainly performed for new plant design, existing plant revamp or expansion, optimal operation, and engineer training.
- Simulation has several advantage like below.
- ① Faster Calculation(More Solutions can be taken at the same time.) ② Accurate Results(rigorous solution can be taken by iteration) ③ Standardization(Simulator has much pure component/binary property Database and thermodynamic methods) ④ Solution of recycle processes(Easy iteration by tearing)

→ **Less Costly than Plant Tests !!**

2. The Structure of Process Simulator



1. Select all of the chemical components that are required in the process from the component database.
2. Select the thermodynamic models required for the simulation. These may be different for different pieces of equipment. For example, to simulate correctly a liquid-liquid extractor, it is necessary to use thermodynamic model that can predict liquid phase activity coefficients and the existence of two liquid phases.
3. Select the topology of flowsheet to be simulated by specifying the input and output streams for each piece of equipment.
4. Select the properties of the feed streams to the process.
5. Select the equipment specifications or parameters.

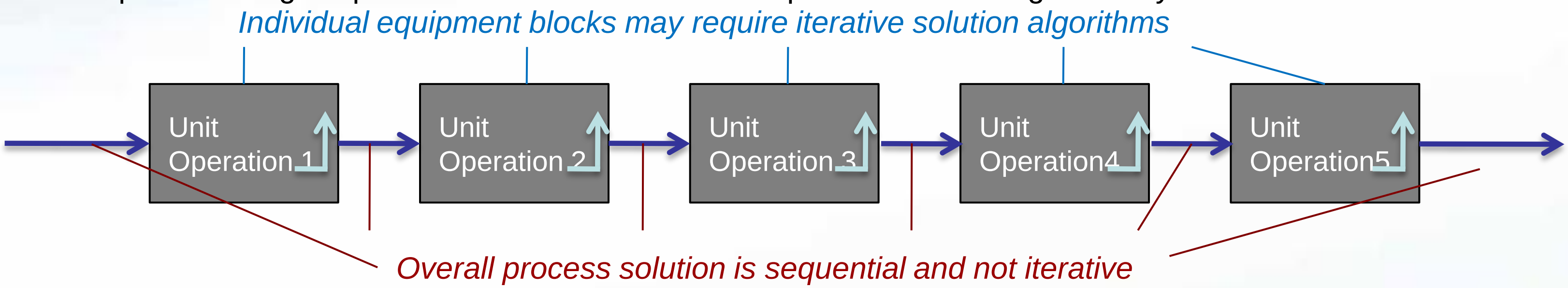
The algorithms for process simulators

- **There are basically three types of solution algorithm for process simulators.**

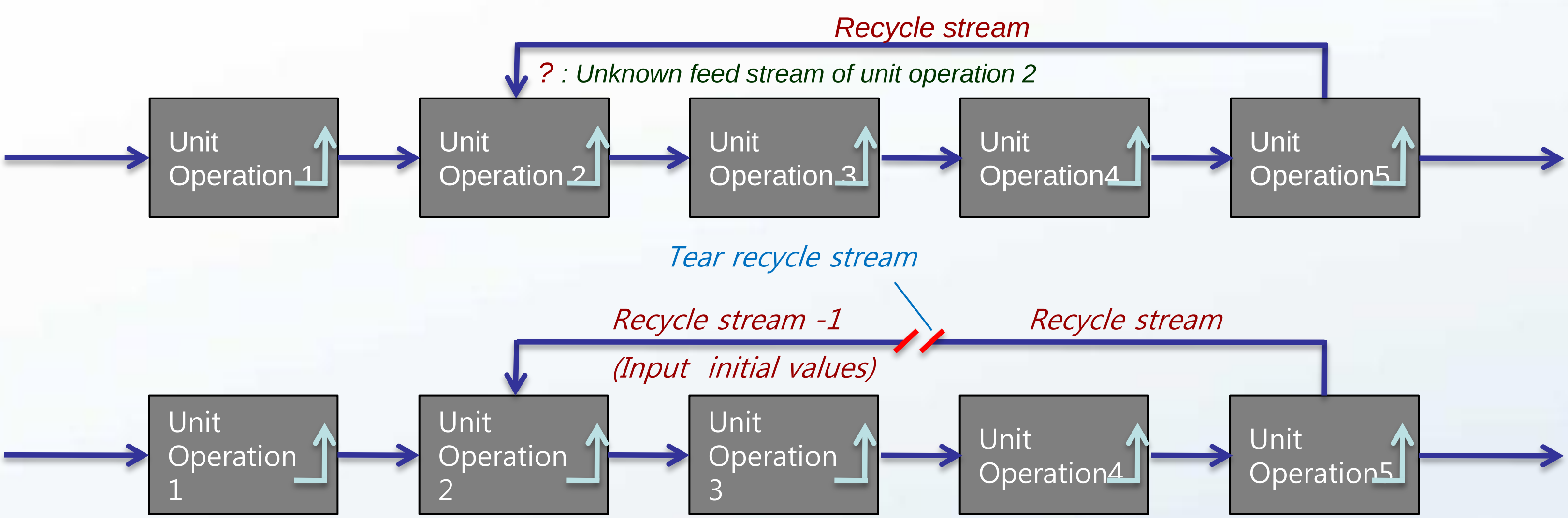
(1) Sequential Modular approach (SM)

: The equations describing the performance of equipment units are grouped together and solved in modules-that is, the process is solved equipment piece by equipment piece.

(a) Solution Sequence Using Sequential Modular Simulator for a process containing No Recycles.



(b) The Use of Tear Streams to solve problems with Recycles Using the Sequential Modular Algorithm



(2) Equation Oriented Non-Module approach (EO Method)

: In the equation solving technique, all the relationships for the process are written out together and then the resulting matrix of nonlinear simultaneous equations is solved to yield the solution. This technique is very efficient in term of computation time but requires a lot of time set up and is unwieldy.

(3) Combined method between SM and EO

The simultaneous modular approach, which combines the modularizing of the equations relating to specific equipment with the efficient solution algorithms for the simultaneous equation solving techniques.

* Of these three types, the sequential modular algorithm is by far the most widely used. In the sequential modular method, each piece of equipment is solved in sequence, starting with the first, followed by second, and so on. It is assumed that all input information required to solve each piece of equipment. Therefore, the output from a given piece of equipment, along with specific information on the equipment, becomes the input to the next piece of equipment in the process. Clearly, for a process without recycle streams, this method requires only one flowsheet iteration to get a converged solution.

II. Unit Operation Solving using Aspen HYSYS

1. Pressure change Equipments
2. Heat Exchangers
3. Distillation Column

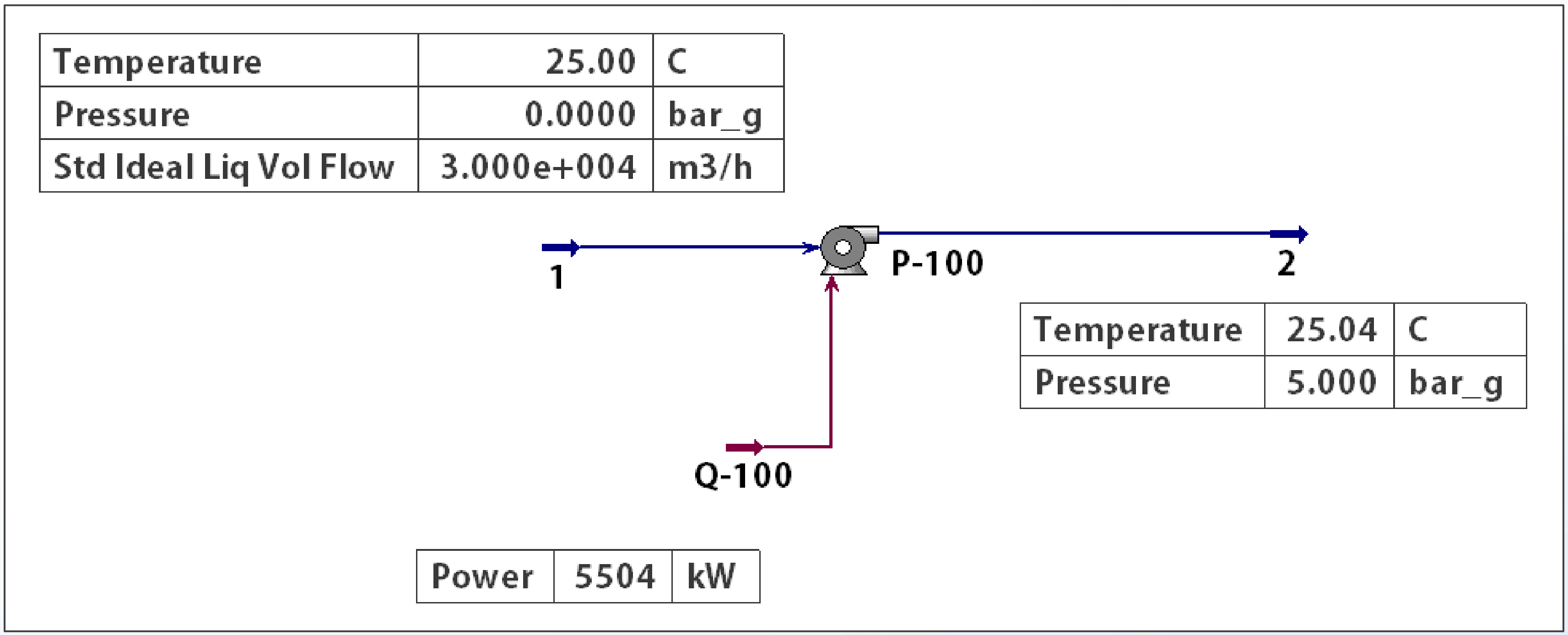
1. Pressure Change Equipments

● **Pumps**

- Problem : “A” Plant is required 25 ^{o}C cooling water to cool down process stream. And, you should try to design the cooling water pump The design value of a pump is like below. Calculate the pump power consumed using Aspen HYSYS.

* Design value; Flow Rate: 30,000 m^3/h, adiabatic efficiency: 75 %(HYSYS Default), Differential pressure: 5 bar

- Solution: Power Consumed = 5504 kW (see below PFD converged by Aspen HYSYS)

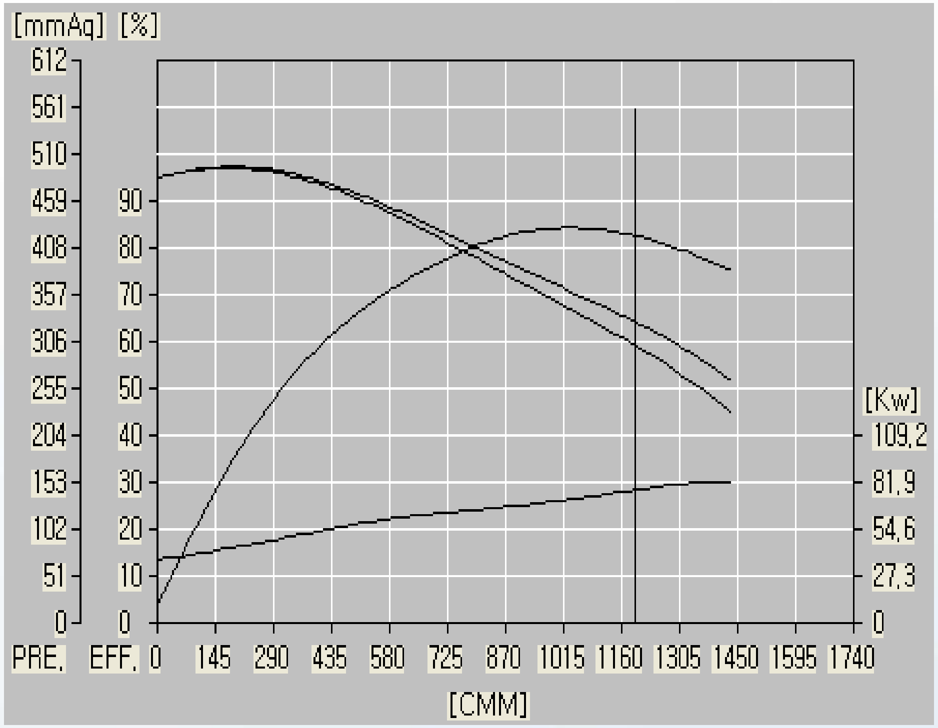


● **Compressor/Blower/Fan**

- Problem : An Air Blower is operated according to the Performance Curve below with 3000 rpm. The Blower leads to less air flow than rated output and causes excessive pressure loss as shown in the figure below. The introduction of inverters is under review to save power. Calculate appropriate rpm and power savings. (The inlet air is assumed at 25 oC and 1 atm)

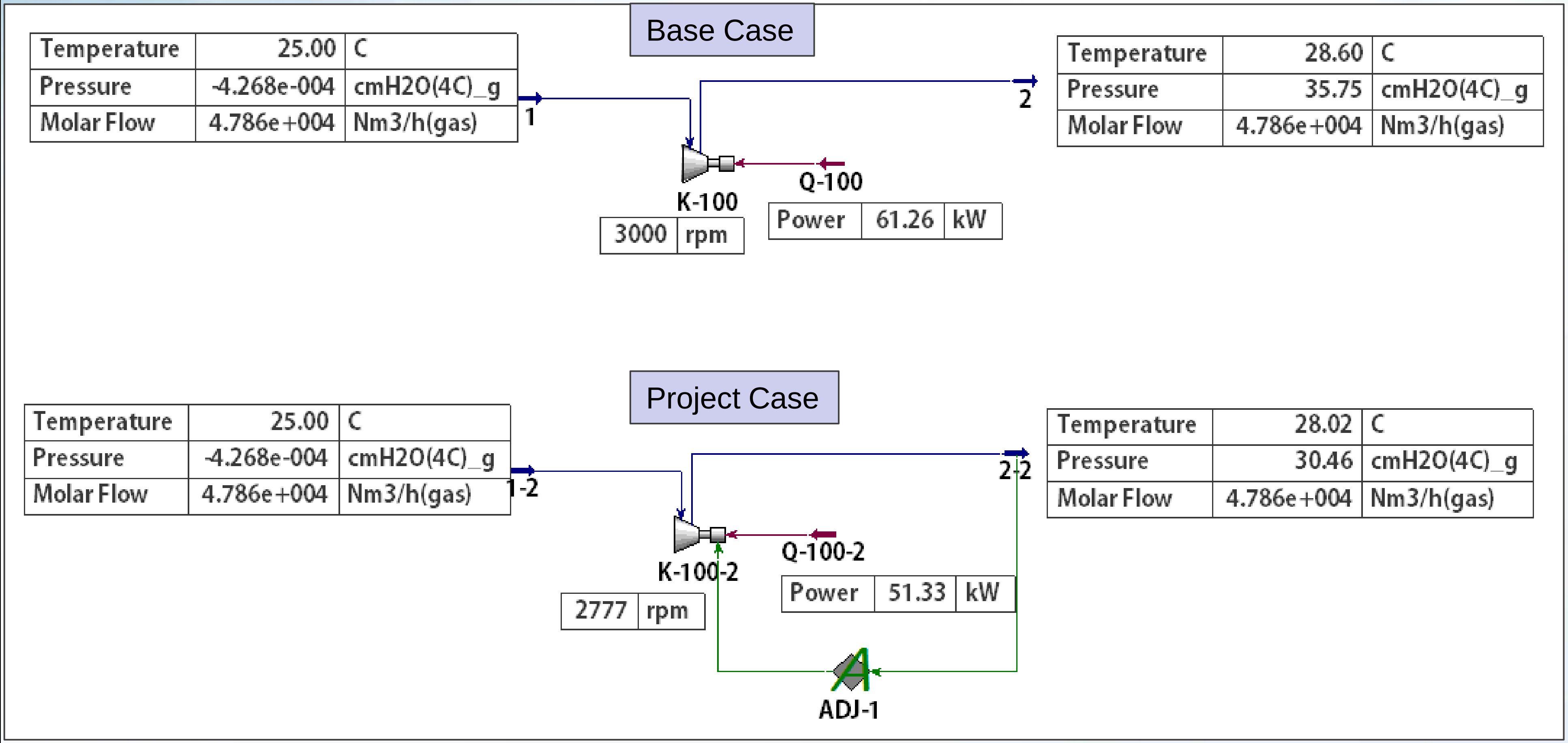
Flow Rate (CMM)	Head (mm-Air)	Efficiency (%)
145	420,000	30
290	419,167	45
435	391,667	62
580	379,167	71
725	354,167	75
870	298,333	82
1,015	295,833	85
1,192	254,167	82
1,305	212,500	80

[FDF Performance Table]



[FDF Performance Curve]

- Solution : The RPM is able to reduce till 2777, and 9.93 kW would be saved from 61.26 kW to 51.33 kW.



2. Heat Exchangers

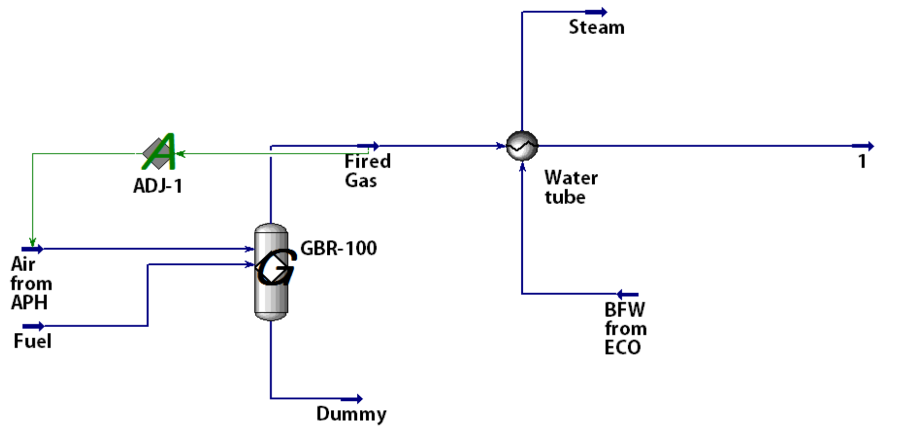
- **Fired Exchanger**

- Problem : "B" Plant have a boiler to generate steam of 15 barg. Natural gas consisted of 85% Methane, 5% Ethane and 10% propane is using for fuel, and ambient air is supplied to combust through the an air preheater to fired box as 190 ºC. BFW is supplied to the boiler as 180 ºC. The temperature of exhaust gas is 550 ºC.
When fuel gas consumed 5,392 kg/h, calculate steam generated rate using Aspen HYSYS.
(at O_2 mol% of flue gas = 5.0, flue gas temperature = 150 ºC, Blow Down rate = 5 t/h)

-Solution : Steam produced 100.3 t/h

Fired Gas		
Temperature	1764	C
Pressure	0.0000	kg/cm2_g
Molar Flow	1.015e+005	Nm3/h(gas)
Master Comp Mole Frac (Oxygen)	0.0507	

Fuel		
Temperature	25.00	C
Pressure	0.0000	kg/cm2_g
Molar Flow	6182	Nm3/h(gas)
Master Comp Mole Frac (Methane)	0.8500	
Master Comp Mole Frac (Ethane)	0.0500	
Master Comp Mole Frac (Propane)	0.1000	



Material Streams								
		Air from APH	Fuel	Fired Gas	BFW from ECO	1	Steam	Dummy
Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	0.0000
Temperature	C	190.0	25.00	1764	180.0	550.0	201.8	1764
Pressure	kg/cm2_g	0.0000	0.0000	0.0000	15.30	0.0000	15.30	0.0000
Molar Flow	Nm3/h(gas)	9.454e+004	6182	1.015e+005	1.247e+005	1.015e+005	1.247e+005	0.0000
Mass Flow	tonne/h	122.2	5.392	127.6	100.3	127.6	100.3	0.0000
Liquid Volume Flow	m3/h	140.5	16.13	151.6	100.5	151.6	100.5	0.0000
Heat Flow	kcal/h	4.791e+006	-5.163e+006	-3.718e+005	-3.642e+008	-4.986e+007	-3.147e+008	-0.0000

- **Shell and tube heat exchanger**

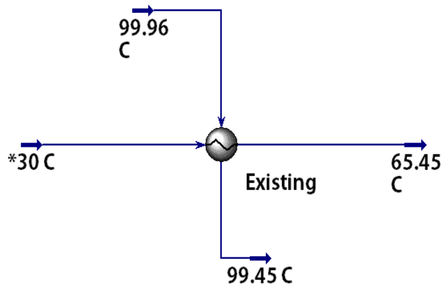
- Problem : Raw water 15 t/h (30 ^{o}C, 5 kg/cm^{2}g) is supplied to make up boiler feed water. You guess that energy loss is occurred in the boiler feed water system since the low water temperature. So you would heat up the raw water by installing an heat exchanger recovered waste heat. Your company have one existing heat exchanger tabled below. How much does the water heat up possible using the heat exchanger. (The waste heat source like below.)
- Moreover, if you install a new heat exchanger and heat the raw water up to 90 ^{o}C, how much does the exchanger be sized?

Existing Heat Exchanger Specification	Waste Heat Source
TEMA Type : H-BEM Size : 585 mmID × 1,829 mmTL, 35.7 m^{2} Baffle Central Spacing : 885 mm Tube ID : 1 inch, Thickness : 2.11mm Tube arrangement : 30 Angle Material : Stainless (SUS316) Fouling resistance : 0.0004 m^{2}-h-C/kcal Allowable pressure drop : 11 kPa (Shell Side) 50 kPa (Tube Side)	Waste Heat Name : Vent Vapor from flash vessel Fluid Composition : 100% H2O Condition : atmospheric saturated steam Flow rate : 2,500 kg/hr

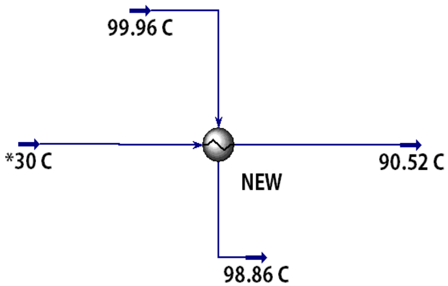
- Solution : The solution can be gotten using process modeling simulator like Aspen Plus or HYSYS integrated Aspen EDR. The solution is next page.

- Solution : In case of using the existing exchanger, 15 t/h raw water of 30 ºC will be heat up to 65.45 ºC recovering 0.55 Gcal/h from waste heat, however, in case of a new exchanger installation and heating up to 90 ºC, the waste heat recovered is 0.94 Gcal/h.

Existing		
Duty	549.1	Mkcal/h
Tube Inlet Temperature	30.00	C
Tube Outlet Temperature	65.45	C
Shell Inlet Temperature	99.96	C
Shell Outlet Temperature	99.45	C



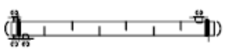
NEW		
Duty	940.2	Mkcal/h
Tube Inlet Temperature	30.00	C
Tube Outlet Temperature	90.52	C
Shell Inlet Temperature	99.96	C
Shell Outlet Temperature	98.86	C



Material Streams									
		Raw Water	Heated Raw Water	Vent Vapor	3	Raw Water-2	Heated Raw Water-2	Vent Vapor-2	3-2
Vapour Fraction		0.0000	0.0000	1.0000	0.5969	0.0000	0.0000	1.0000	0.3105
Temperature	C	30.00	65.45	99.96	99.45	30.00	90.52	99.96	98.86
Pressure	kg/cm2_g	5.000	4.970	2.022e-007	-1.871e-002	5.000	4.570	2.022e-007	-4.003e-002
Molar Flow	kgmole/h	832.6	832.6	138.8	138.8	832.6	832.6	138.8	138.8
Mass Flow	tonne/h	15.00	15.00	2.500	2.500	15.00	15.00	2.500	2.500
Liquid Volume Flow	m3/h	15.03	15.03	2.505	2.505	15.03	15.03	2.505	2.505
Heat Flow	Mkcal/h	-5.688e+004	-5.633e+004	-7939	-8488	-5.688e+004	-5.594e+004	-7939	-8879

Heat Exchanger Specification Sheet

1	Company:					
2	Location:					
3	Service of Unit: Our Reference:					
4	Item No.: Your Reference:					
5	Date: Rev No.: Job No.:					
6	Size: 438 - 5850 mm Type: BEM Horizontal				Connected in: 1 parallel 1 series	
7	Surf/unit(eff.) 40 m²		Shells/unit 1		Surf/shell(eff.) 40 m²	
8	**PERFORMANCE OF ONE UNIT**					
9	Fluid allocation		Shell Side		Tube Side	
10	Fluid name		Vent Vapor-2->3-2		Raw Water-2->Heated Raw Water-2	
11	Fluid quantity, Total	kg/h	2500		15000	
12	Vapor (In/Out)	kg/h	2500	776	0	0
13	Liquid	kg/h	0	1724	15000	15000
14	Noncondensable	kg/h	0	0	0	0
15						
16	Temperature (In/Out)	°C	99.96	98.86	30	90.52
17	Dew / Bubble point	°C	99.96	99.96	158.32	158.32
18	Density Vapor/Liquid	kg/m³	0.59 /	0.57 / 949.38	/ 1003.72	/ 955.99
19	Viscosity	cp	0.0121 /	0.0121 / 0.2843	/ 0.7972	/ 0.3095
20	Molecular wt, Vap		18.02	18.02		
21	Molecular wt, NC					
22	Specific heat	kJ/(kg-K)	1.907 /	1.906 / 4.393	/ 4.313	/ 4.376
23	Thermal conductivity	W/(m-K)	0.0245 /	0.0244 / 0.6799	/ 0.6182	/ 0.6762
24	Latent heat	kJ/kg	2276.4	2279.4		
25	Pressure (abs)	kPa	101.325	97.399	591.658	549.529
26	Velocity (Mean/Max)	m/s	10.26 / 35.37		1.22 / 1.54	
27	Pressure drop, allow./calc.	kPa	11	3.926	50.014	42.128
28	Fouling resistance (min)	m²-K/W	0.00034		0.00034	0.00041 Ao based
29	Heat exchanged 1092.7	kW			MTD (corrected) 29.22	°C
30	Transfer rate, Service 934.9		Dirty 935		Clean 3187	W/(m²-K)

31	**CONSTRUCTION OF ONE SHELL**					**Sketch**
32				Shell Side	Tube Side	
33	Design/Vacuum/test pressure		kPa	300 / /	700 / /	
34	Design temperature		°C	135	125	
35	Number passes per shell			1	8	
36	Corrosion allowance		mm	3.18	3.18	
37	Connections	In	mm	1 202.72 / -	1 52.5 / -	
38	Size/Rating	Out		1 154.05 / -	1 52.5 / -	
39	ID	Intermediate		/ -	/ -	

3. Distillation Column

● Distillation Column

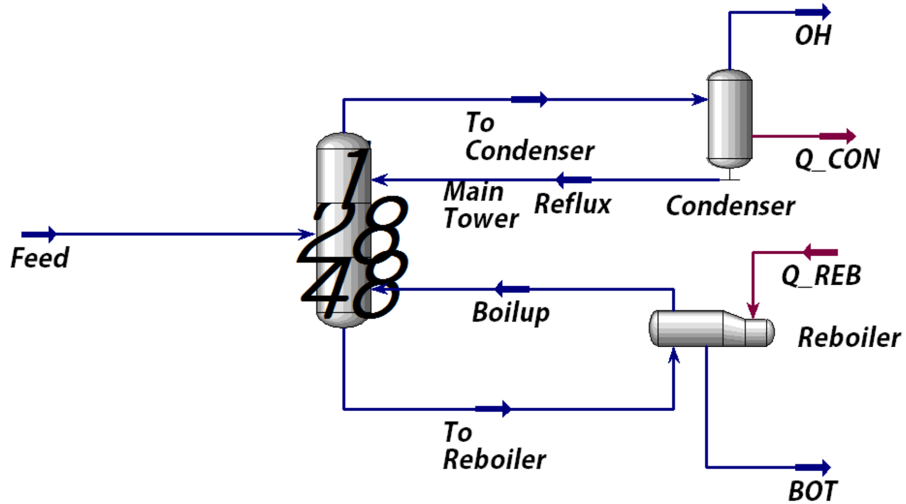
- Problem : Light composition in the process stream that is composed of C4-C8 is fully refluxed with vapor in the distillation column and the composition containing C6 and greater components is being produced at the bottom of the column. At this time, n-Pentane is controlled at 0.1wt% at the bottom of the column and n-Hexane controlled on-spec at 0.05 wt% at the top of the column. Hence, a feed/bottom heat exchanger is to reduce heat duty of the distillation column reboiler by increasing feed temperature.

Set up the simulation model about this distillation column.

Feed Stream Composition	Stream Condition	Distillation Column Data
n-Butane 5 wt% n-Pentane 10 wt% n-Hexane 60 wt% n-Heptane 15 wt% n-Octane 10 wt%	Pressure: 4 kg/cm^2g Temperature: 50°C Flow: 50 ton/h	No. of Stage 48 Valve Tray Feed Stage: 28 stage Condenser Pressure: 3.4 kg/cm^2g Condenser DP : 0.1 bar Column Bottom Pressure: 3.8 kg/cm^2g Reboiler DP : 0.15 bar

● Distillation Column

- Solution



Material Streams								
		Reflux	To Condenser	Boilup	To Reboiler	OH	BOT	Feed
Vapour Fraction		0.0000	1.0000	1.0000	0.0000	1.0000	0.0000	0.0000
Temperature	C	75.79	80.97	136.8	132.5	75.79	136.8	50.00
Pressure	kg/cm2_g	3.400	3.502	3.800	3.647	3.400	3.800	4.000
Molar Flow	kgmole/h	275.6	387.3	714.1	1181	111.8	467.3	579.0
Mass Flow	kg/h	1.910e+004	2.656e+004	6.309e+004	1.056e+005	7461	4.254e+004	5.000e+004
Liquid Volume Flow	m3/h	30.74	42.91	94.62	158.0	12.16	63.34	75.51
Heat Flow	Mkcal/h	-1.049e+004	-1.255e+004	-2.616e+004	-5.098e+004	-3572	-2.033e+004	-2.687e+004

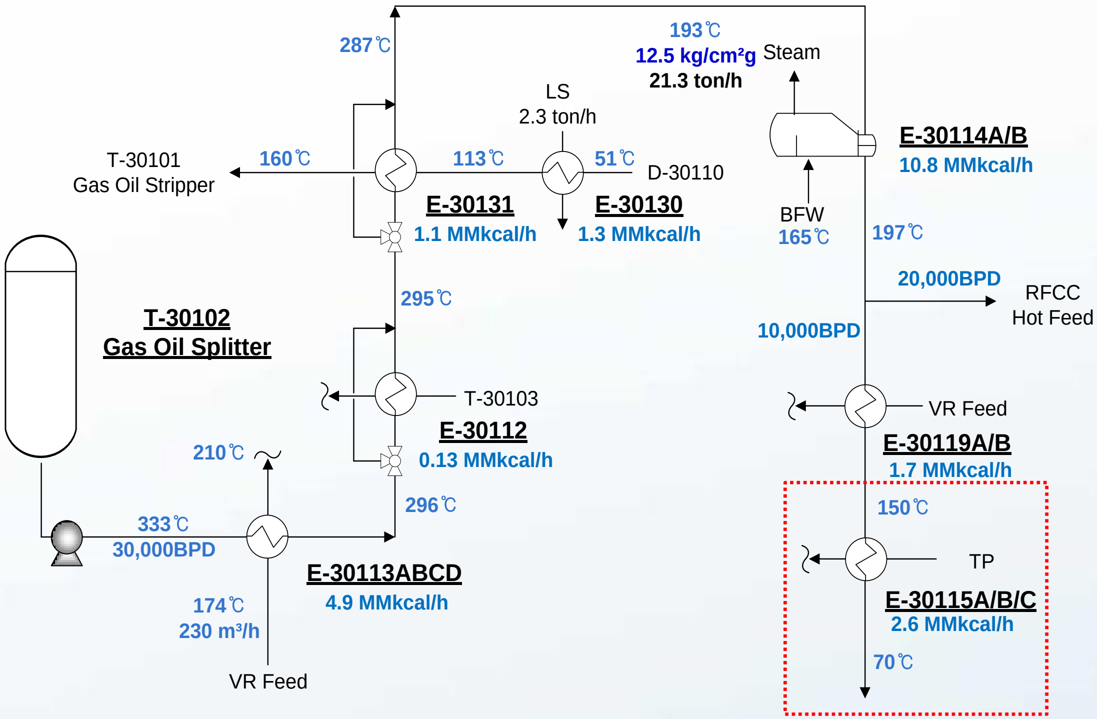
III. Energy consulting example using Aspen HYSYS

1. Gasoil stripper
2. Waste heat boiler
3. Phenol Process

1. GasOil stripper

- **Base Case PFD**

- The bottom temperature of 'GasOil Splitter' is 333℃. It should be cooled before storage tank. In the heat recovery process, the feed stream(VR Feed) is heated up to 210℃ and middle pressure steam is generated at the steam generator.
- Energy Loss Point : The energy loss is occurred at the 'Tempered Water Cooler'. The steam temperature before TW Cooler is 150℃. It is enough to heat other steam up to 120~130℃(In this sample case, target approach temperature is 25℃).



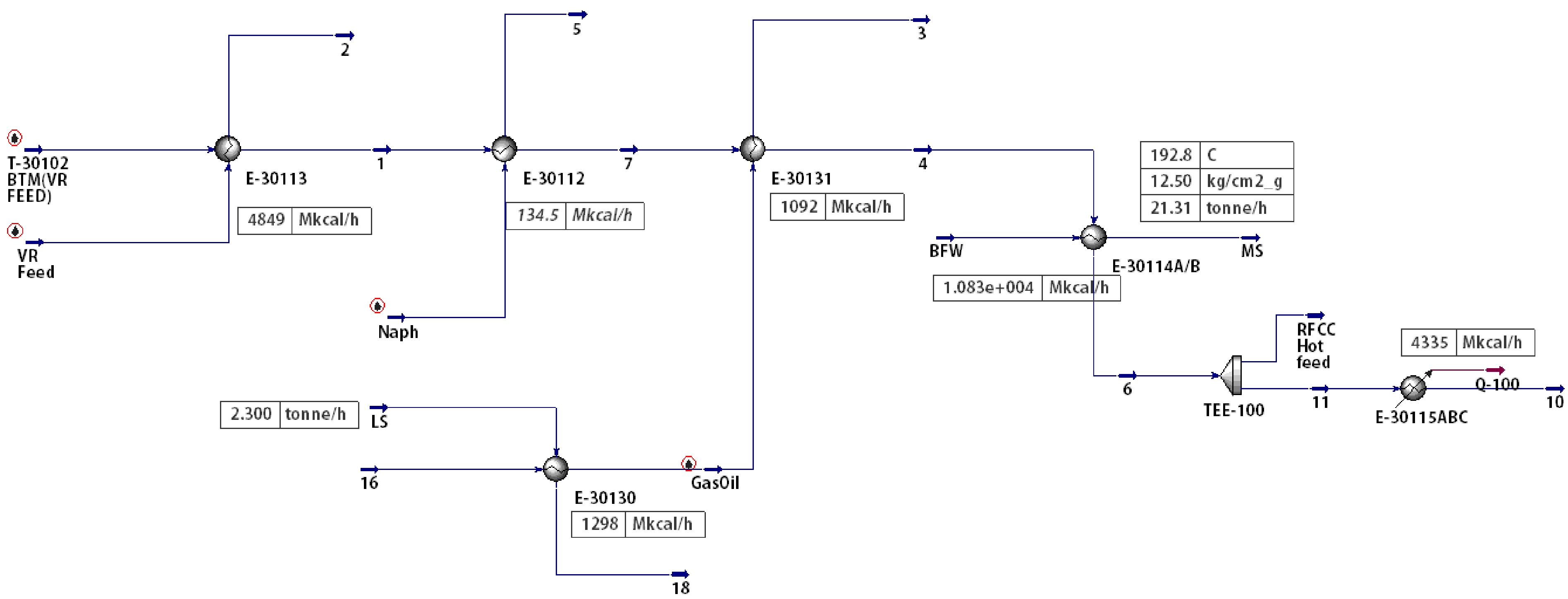
- **Process Modeling for base case using Aspen HYSYS**

- Process Modeling Condition

Boiler Feed Water : 165℃, 3.5kg/cm^2·g

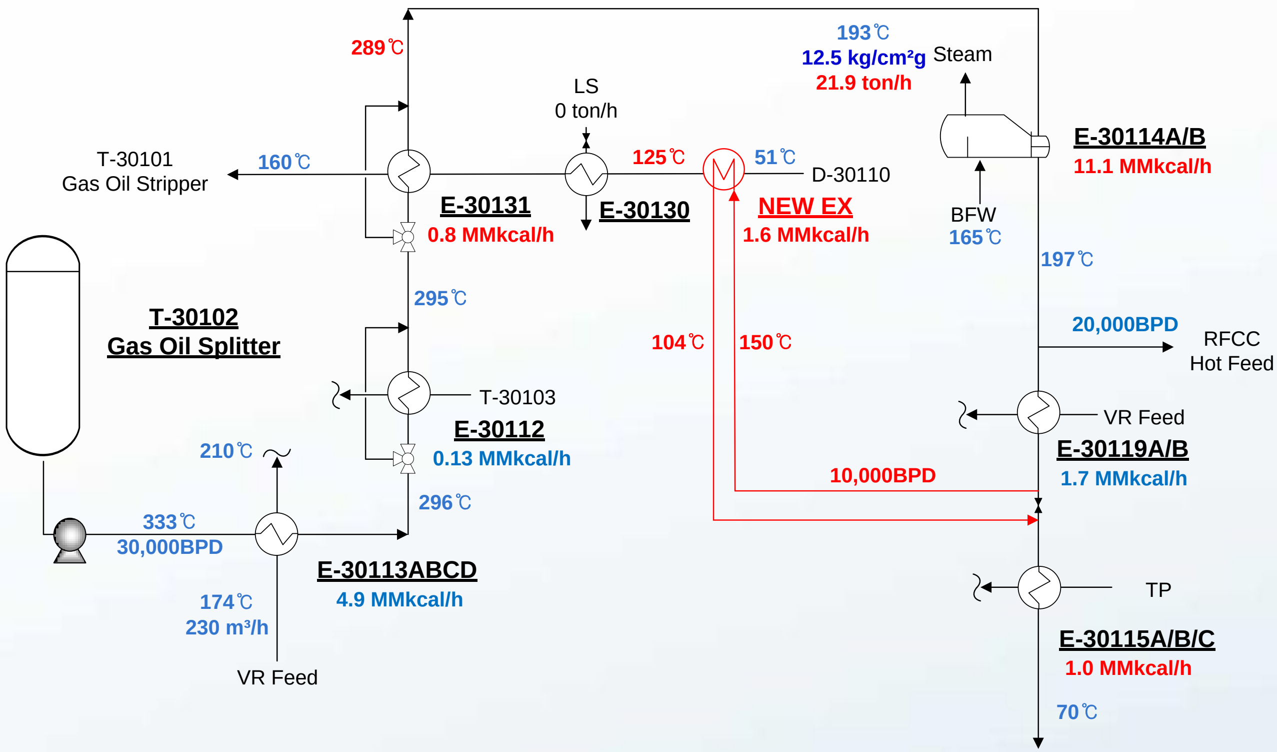
Middle Pressure Steam : 193℃, 12.5kg/cm^2·g

Stripper Bottom Feed, VR Feed, Naphtha and Gas Oil steams are generated by process simulator(Aspen HYSYS Oil manager)(based on lab distillation data.)

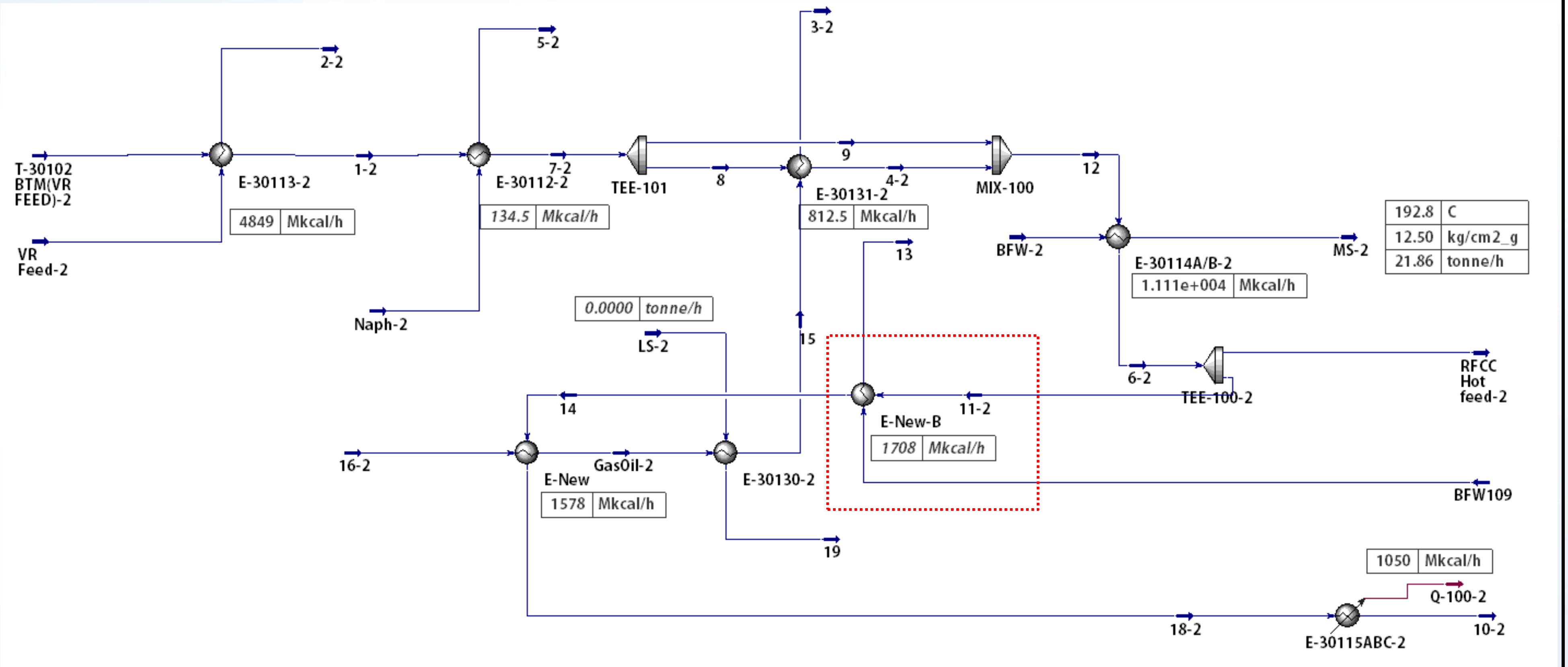


● Project Case PFD

- Energy Saving Target : The ‘GasOil stripper feed’ is heated by low pressure steam. If it heated by waste heat, it can save the LP steam(definitely, it can save fuel gas or oil at the steam boiler
- Run-down stream have enough heat amount to heat up this feed stream. In this case, we set the target heat up temperature 125℃. It is typical approach temperature in refinery heat exchanger network design.
- The expected effect of applying project case is saving LP steam about 2.3 ton/h and increasing MP Steam generation about 0.6 ton/h.



- **Process Modeling for project case using Aspen HYSYS**



- **New heat exchanger design for project case using Aspen EDR**

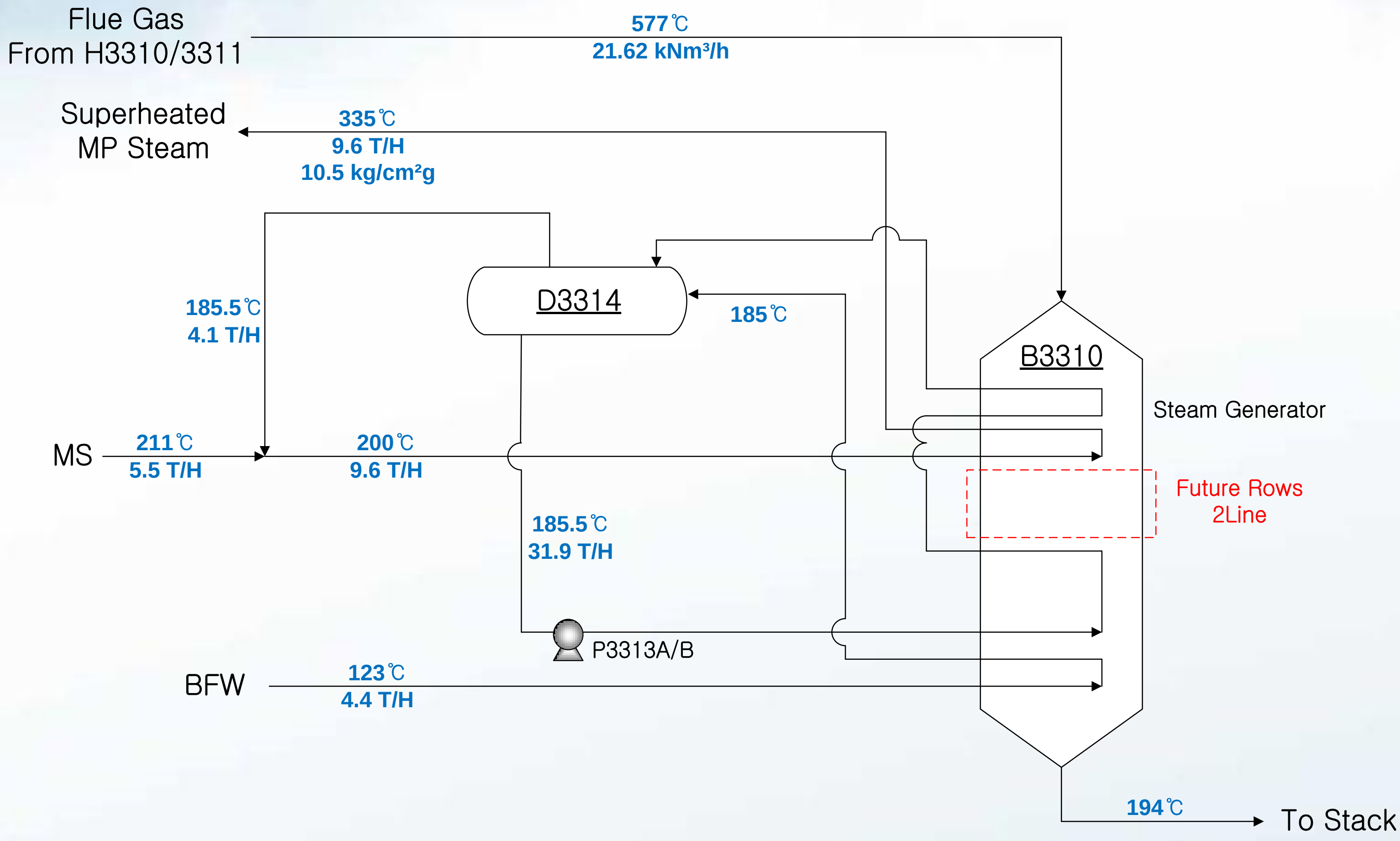
Size: 600 - 6000 mm	Type: AES Horizontal	Connected in: 1 parallel 2 series			
Surf/unit(eff.) 206 m²	Shells/unit 2	Surf/shell(eff.) 103 m²			
PERFORMANCE OF ONE UNIT					
Fluid allocation		Shell Side		Tube Side	
Fluid name		14->18-2		16-2->GasOil-2	
Fluid quantity, Total	kg/h	62277		42780	
Vapor (In/Out)	kg/h	0	0	0	0
Liquid	kg/h	62277	62277	42780	42780
Noncondensable	kg/h	0	0	0	0
Temperature (In/Out)	°C	150.15	103.46	50.7	125.57
Dew / Bubble point	°C				
Density Vapor/Liquid	kg/m³	/ 848.99	/ 880.82	/ 833.29	/ 780.47
Viscosity	cp	/ 7.87	/ 21.7149	/ 2.1183	/ 0.6702
Molecular wt, Vap					
Molecular wt, NC					
Specific heat	kJ/(kg-K)	/ 2.36	/ 2.176	/ 1.898	/ 2.222
Thermal conductivity	W/(m-K)	/ 0.1187	/ 0.1252	/ 0.1179	/ 0.1088
Latent heat	kJ/kg				
Pressure (abs)	kPa	2160.722	2115.983	2258.789	2230.831
Velocity (Mean/Max)	m/s	0.45 / 0.58		0.74 / 0.77	
Pressure drop, allow./calc.	kPa	50	44.739	50	27.957
Fouling resistance (min)	m²-K/W	0		0	0 Ao based
Heat exchanged 1833. kW		MTD (corrected) 31.71 °C			
Transfer rate, Service 280		Dirty 280.6		Clean 280.6	W/(m²-K)

CONSTRUCTION OF ONE SHELL				Sketch
		Shell Side	Tube Side	
Design/Vacuum/test pressure	kPa	2400 / /	2500 / /	
Design temperature	°C	190	165	
Number passes per shell		1	4	
Corrosion allowance	mm	3.18	3.18	
Connections	In mm	1 154.05 / -	1 77.93 / -	
Size/Rating	Out	1 154.05 / -	1 90.12 / -	
ID	Intermediate	1 154.05 / -	1 77.93 / -	

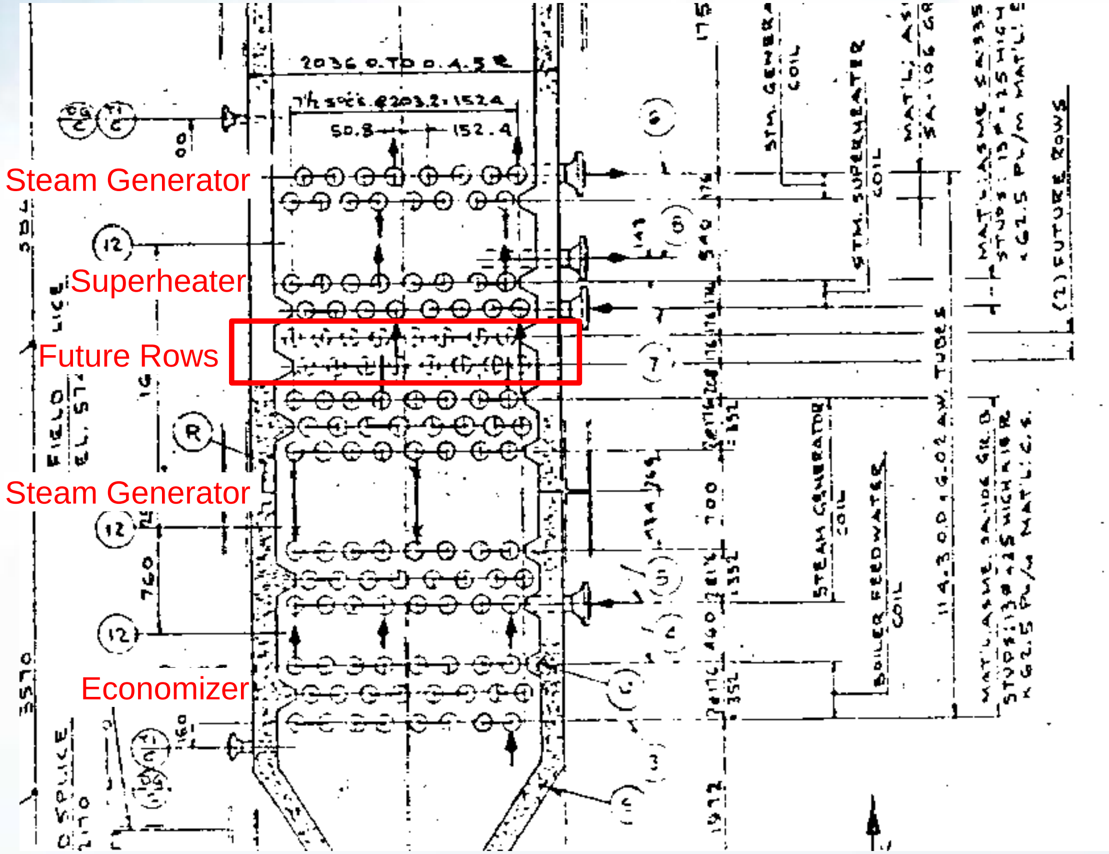
Tube No. 226 OD 25.4 TksAverage 2.11 mm Length 6000 mm Pitch 31.75 mm			
Tube type Plain #/m Material Carbon Steel		Tube pattern 30	
Shell Carbon Steel ID 600 OD 620 mm		Shell cover	Carbon Steel
Channel or bonnet	Carbon Steel	Channel cover	Carbon Steel
Tubesheet-stationary	Carbon Steel -	Tubesheet-floating	Carbon Steel
Floating head cover	Carbon Steel	Impingement protection	None
Baffle-cross Carbon Steel Type Single segmental Cut(%d) 29.37 Horiz		Spacing: c/c 235 mm	
Baffle-long - Seal Type		Inlet 388.71 mm	
Supports-tube U-bend 0 Type			
Bypass seal	Tube-tubesheet joint	Expanded only (2 grooves)(App.A 'i')	
Expansion joint -	Type	None	
RhoV2-Inlet nozzle 1015	Bundle entrance 122	Bundle exit 117	kg/(m-s²)
Gaskets - Shell side	Flat Metal Jacket Fibe	Tube side	Flat Metal Jacket Fibe
Floating head	Flat Metal Jacket Fibe		
Code requirements	ASME Code Sec VIII Div 1	TEMA class	R - refinery service
Weight/Shell	4270.4 Filled with water 6016.5	Bundle	2033.4 kg

2. Waste heat boiler Heat

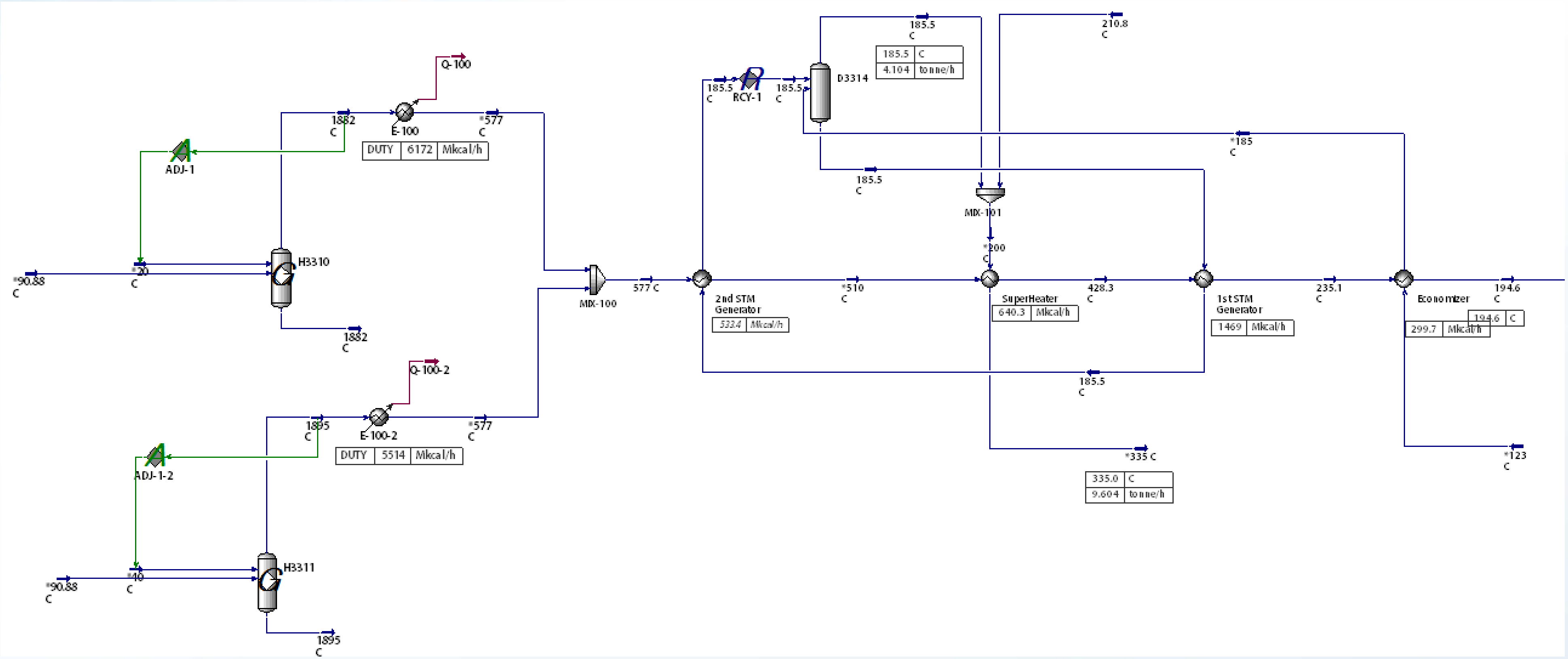
- **Base Case PFD**



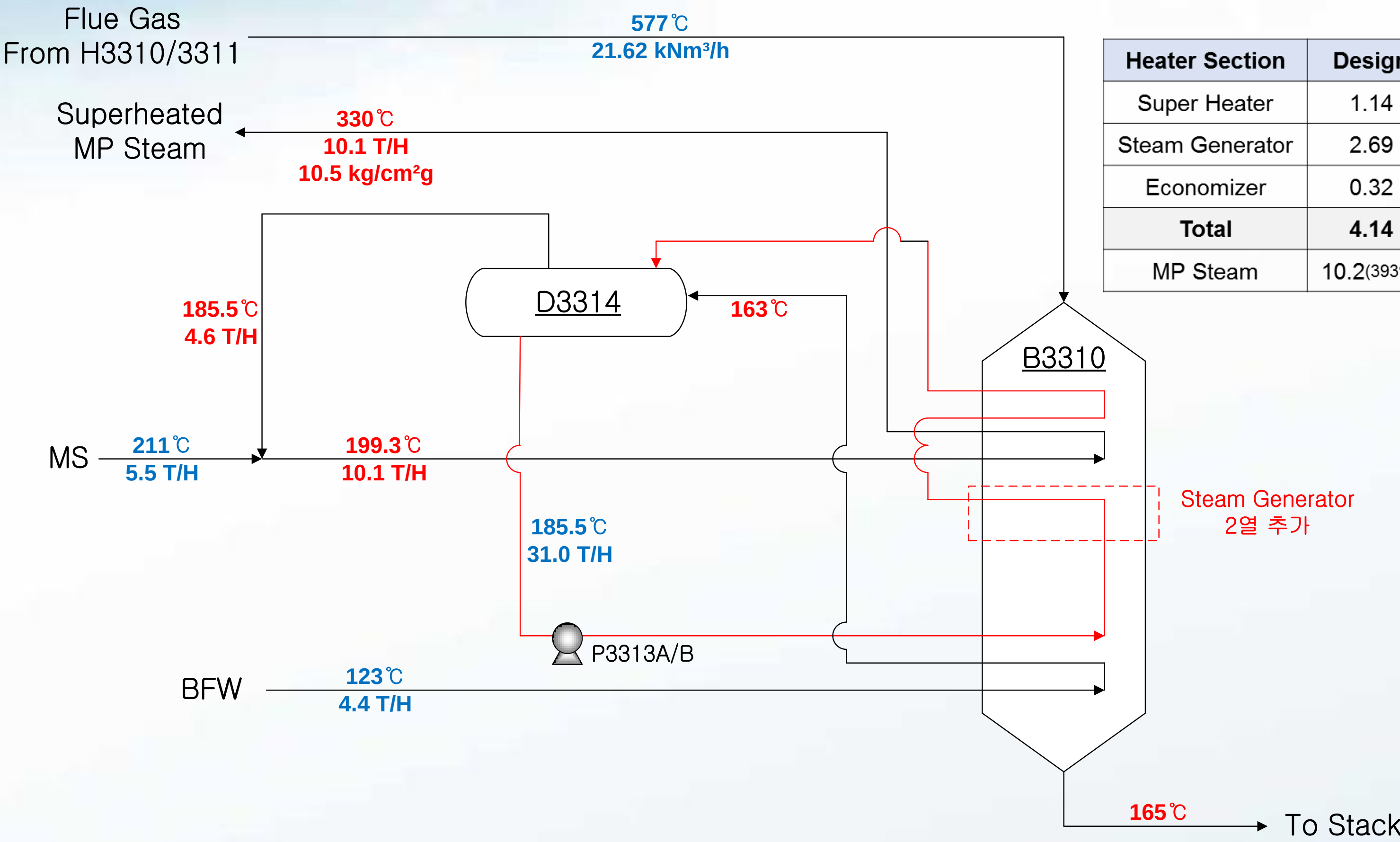
- **Elevation drawing of WHB**



- **Process Modeling for base case using Aspen HYSYS**



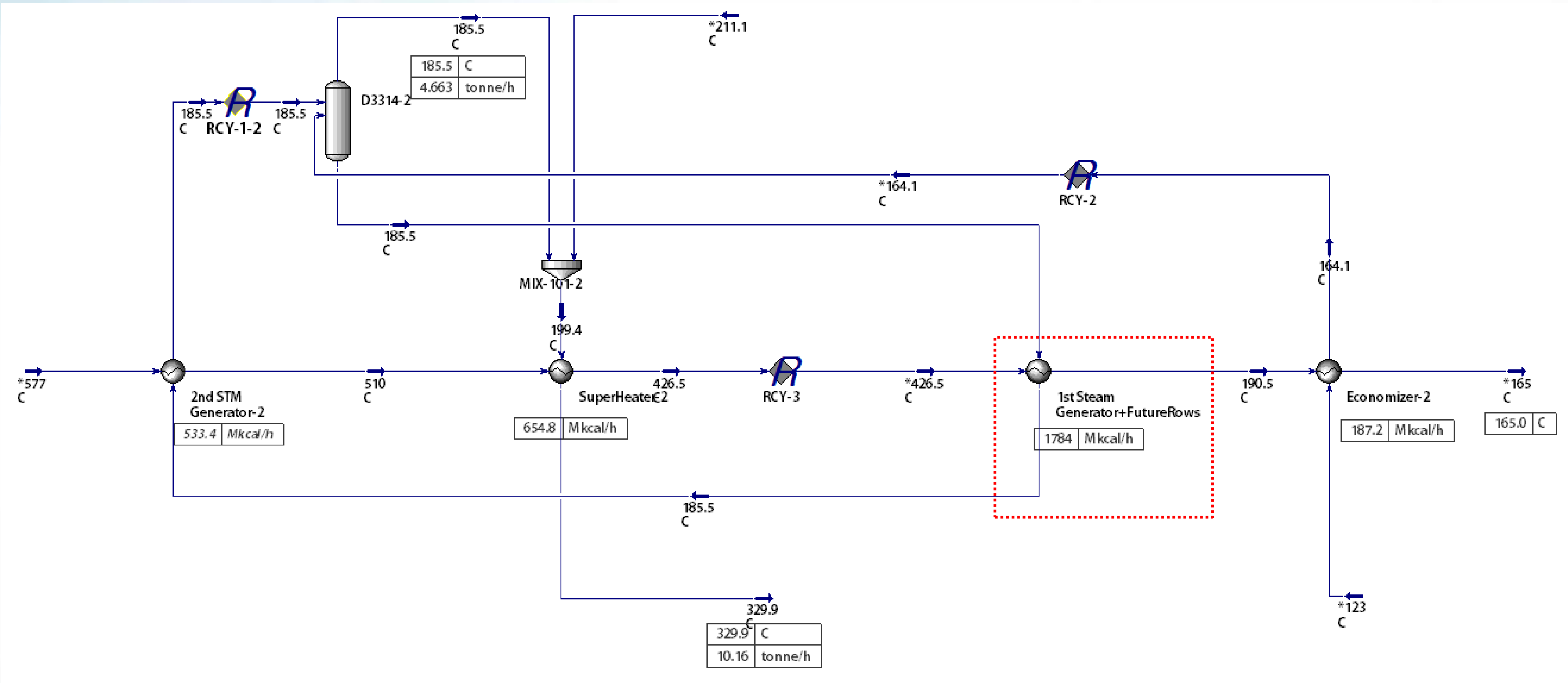
● Project Case PFD



(Unit : MMkcal/h, t/h)

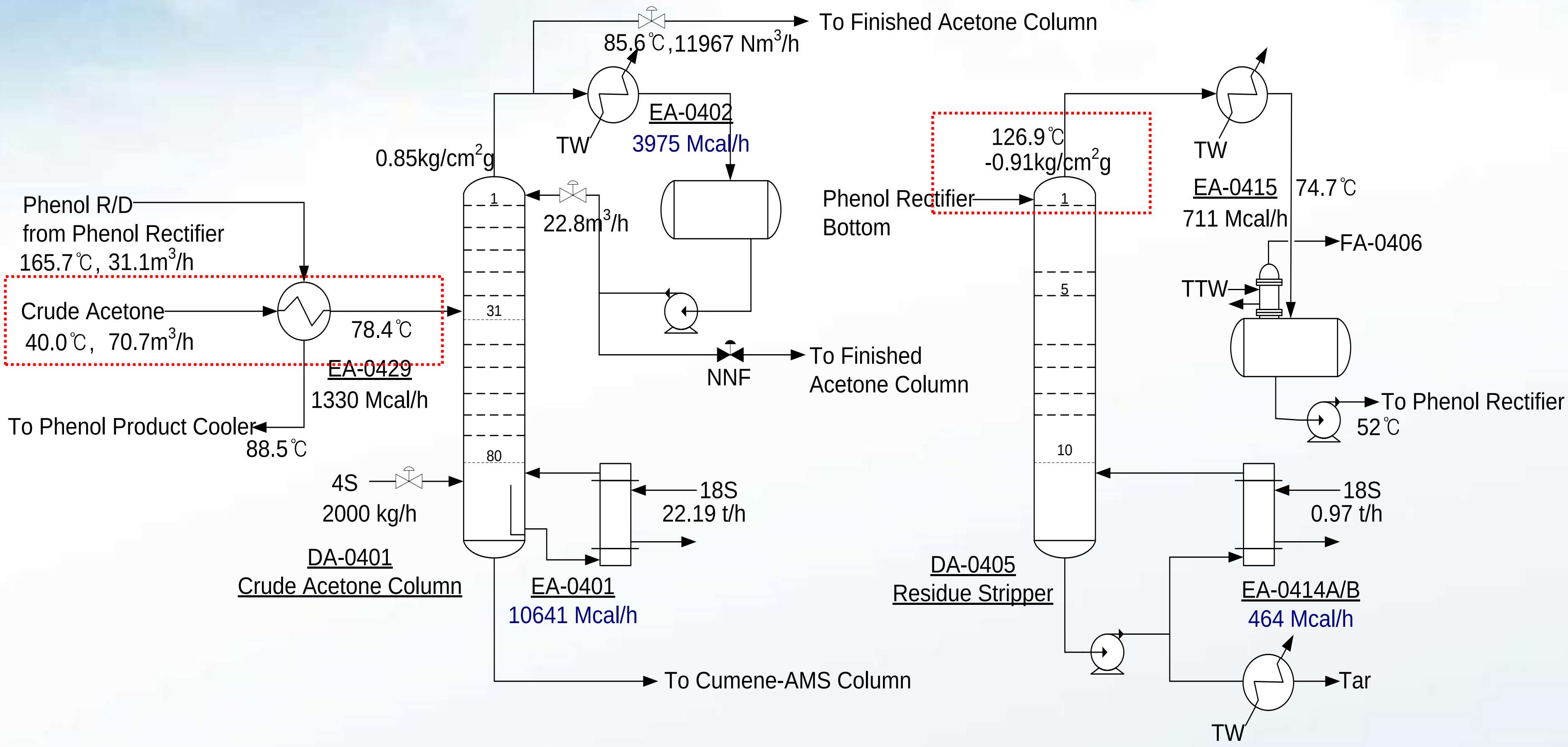
Heater Section	Design	As is	To be	Difference
Super Heater	1.14	0.64	0.65	0.01
Steam Generator	2.69	2.00	2.32	0.32
Economizer	0.32	0.30	0.19	-0.11
Total	**4.14**	**2.94**	**3.16**	0.22
MP Steam	10.2(393℃)	9.6	10.1	0.5

- **Process Modeling for project case using Aspen HYSYS**

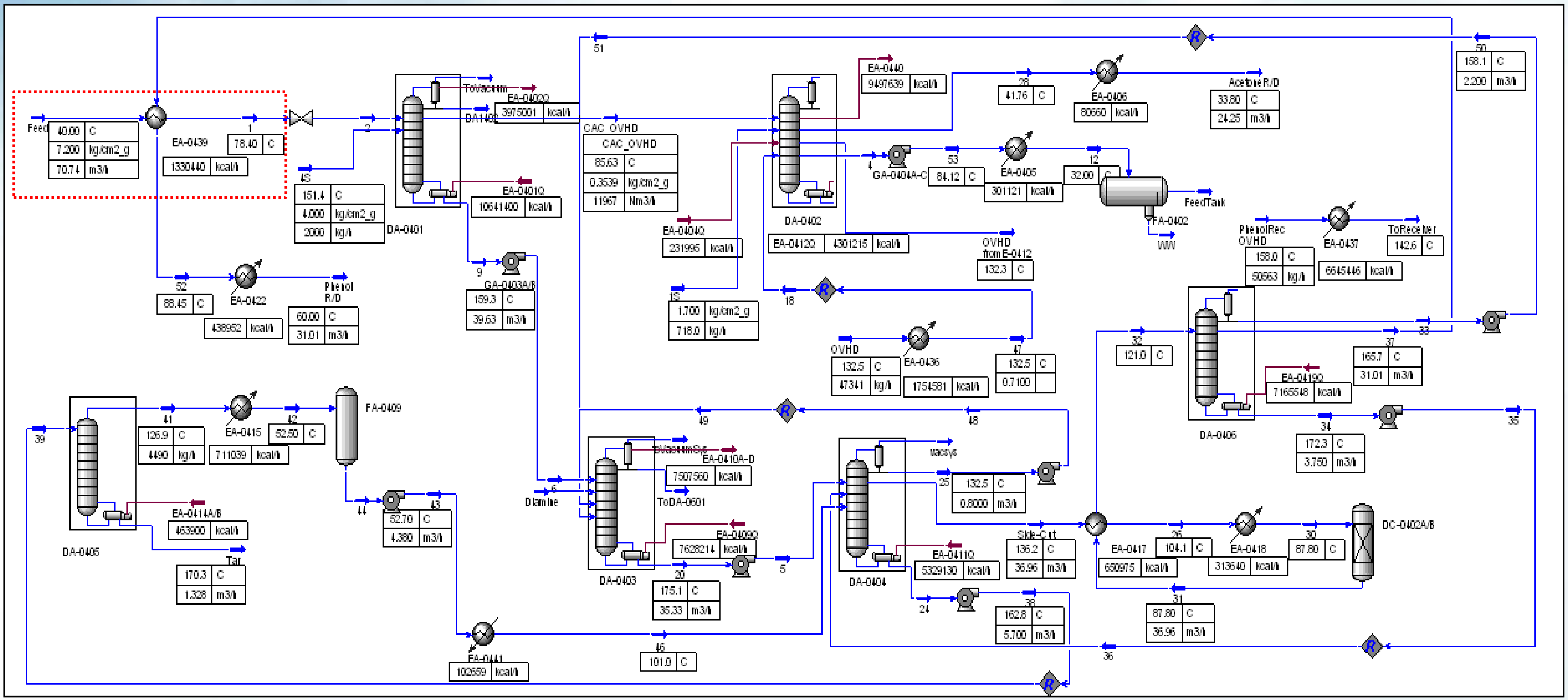


3. Phenol Process

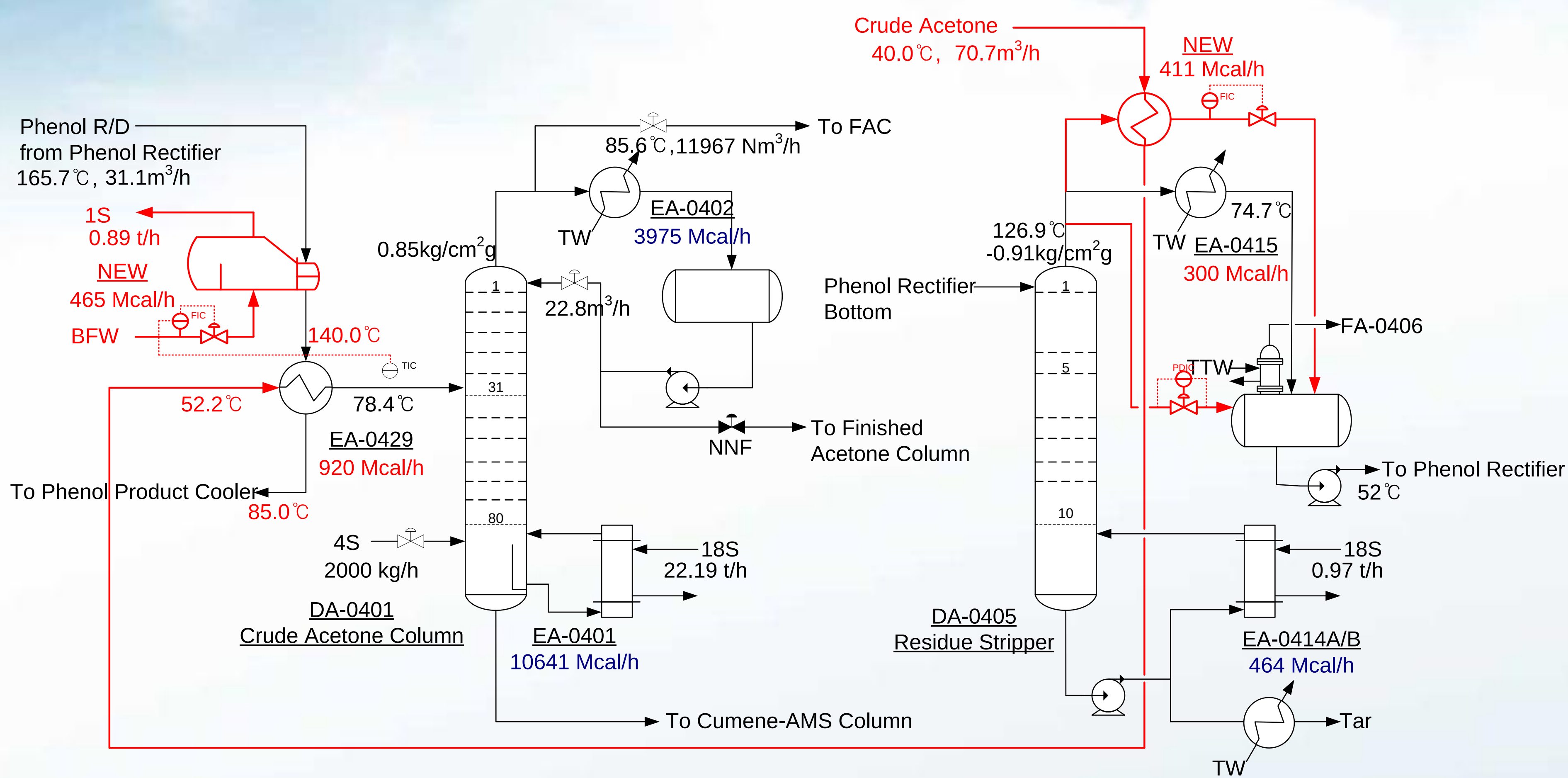
- **Base Case PFD**



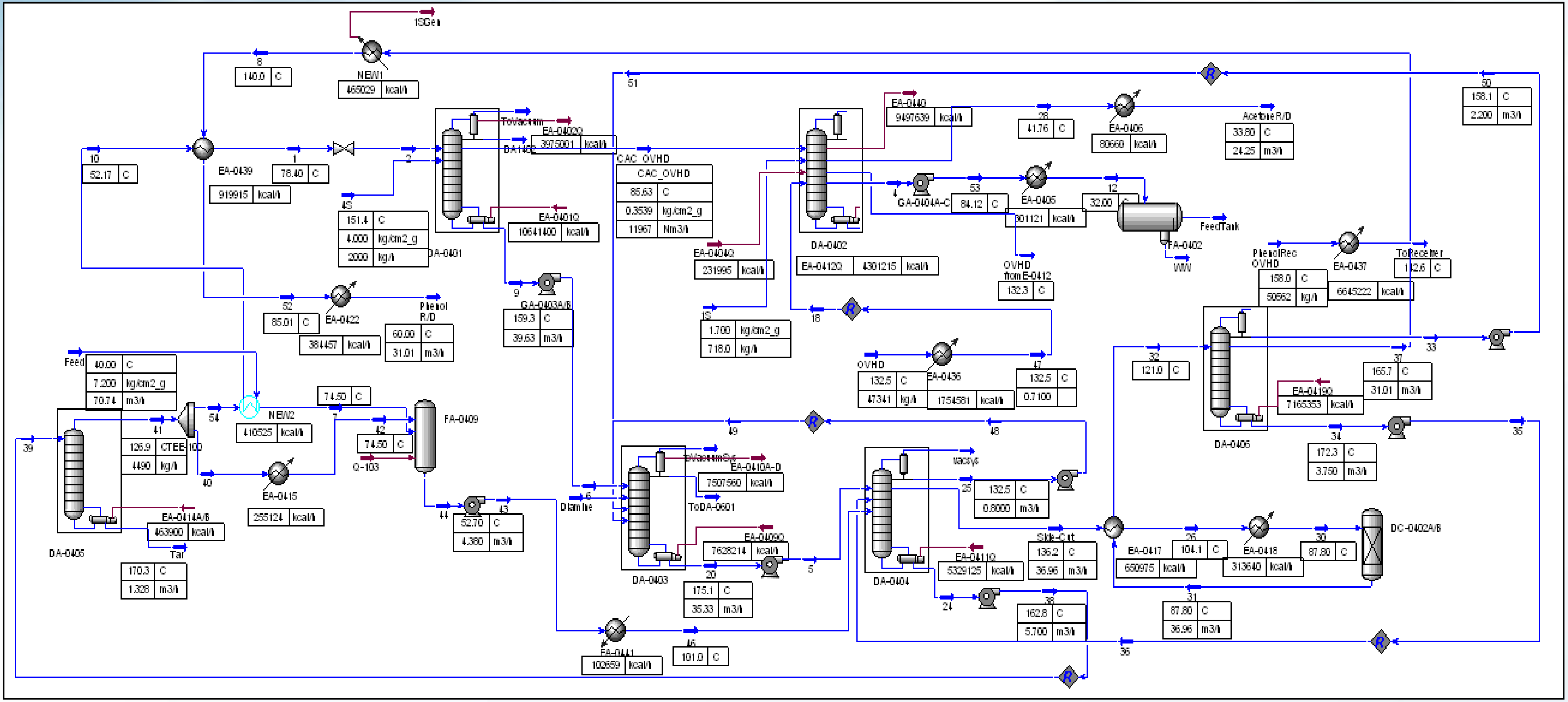
- **Process Modeling for base case using Aspen HYSYS**



● Project Case PFD



- **Process Modeling for project case using Aspen HYSYS**



Thank you!

한국에너지공단
KOREA ENERGY AGENCY