
ISS(Isotope Separation System)

초저온증류 공정시뮬레이션

공주대학교 화학공학부

조 정 호

목 차

1. ISS(Isotope Separation System) 소개
2. ITER ISS 평형 반응기
3. 헬륨 냉동 사이클
4. Pure Component Properties
5. ITER ISS 공정 시뮬레이션 Case 1
6. ITER ISS 공정 시뮬레이션 Case 2
7. ITER ISS 공정 시뮬레이션 Case 3

5. ITER ISS 공정 시뮬레이션

Case 1

5. ITER ISS 공정 시뮬레이션 Case 1

➤ Feedstock Information

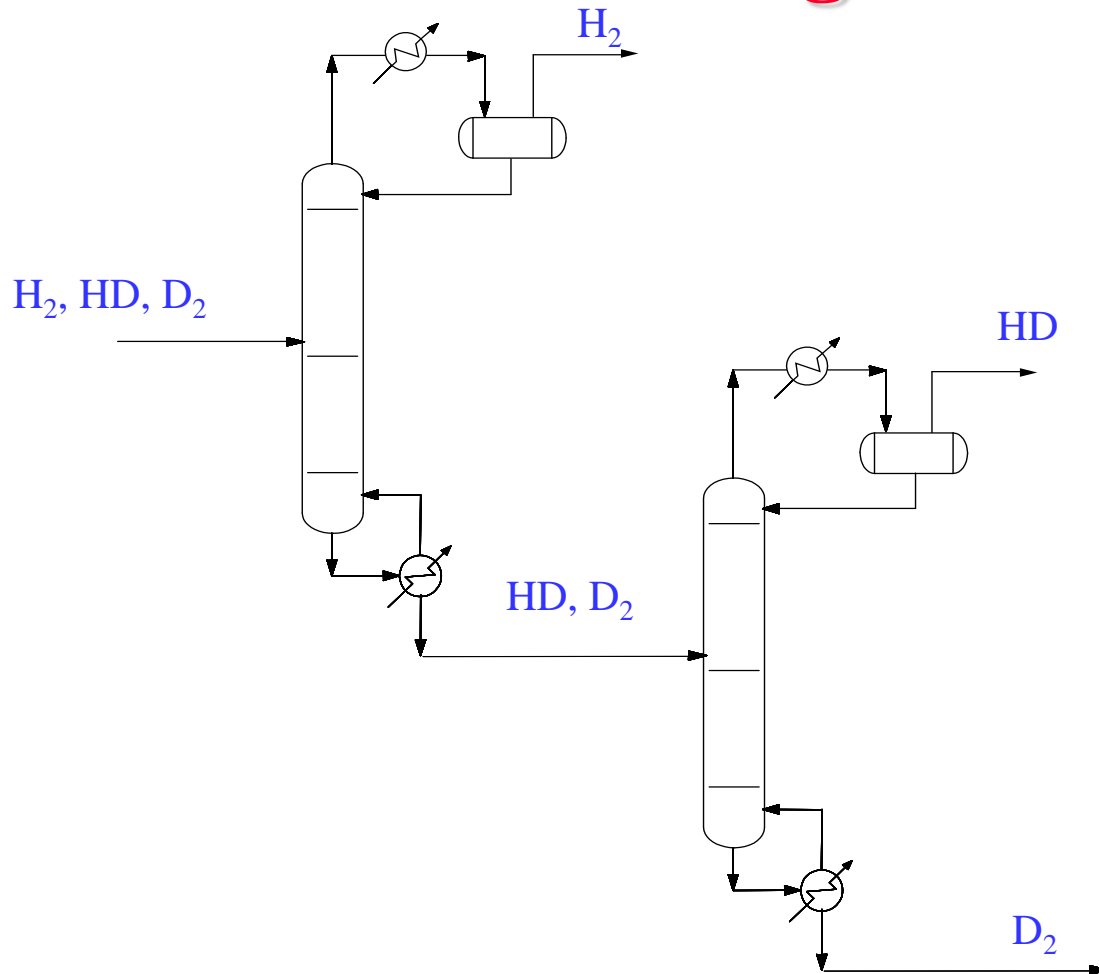
Component	Mole%
H ₂	30.0
HD	30.0
D ₂	40.0
Flow (kmol/hr)	100.0
Temp. (K)	30.0
Press (kPa)	120.0

Cold Utility Condition

- 1st Refrigerant: Liquid Helium
 - Critical Temperature: 5.21 K
 - Normal Boiling Temperature: 4.22 K
 - Supply Temperature: Should be lower than T_c of He.

- 2nd Refrigerant: Liquid Nitrogen

Distillation Column Configuration



Separation Column Operating Condition

➤ 1st Column

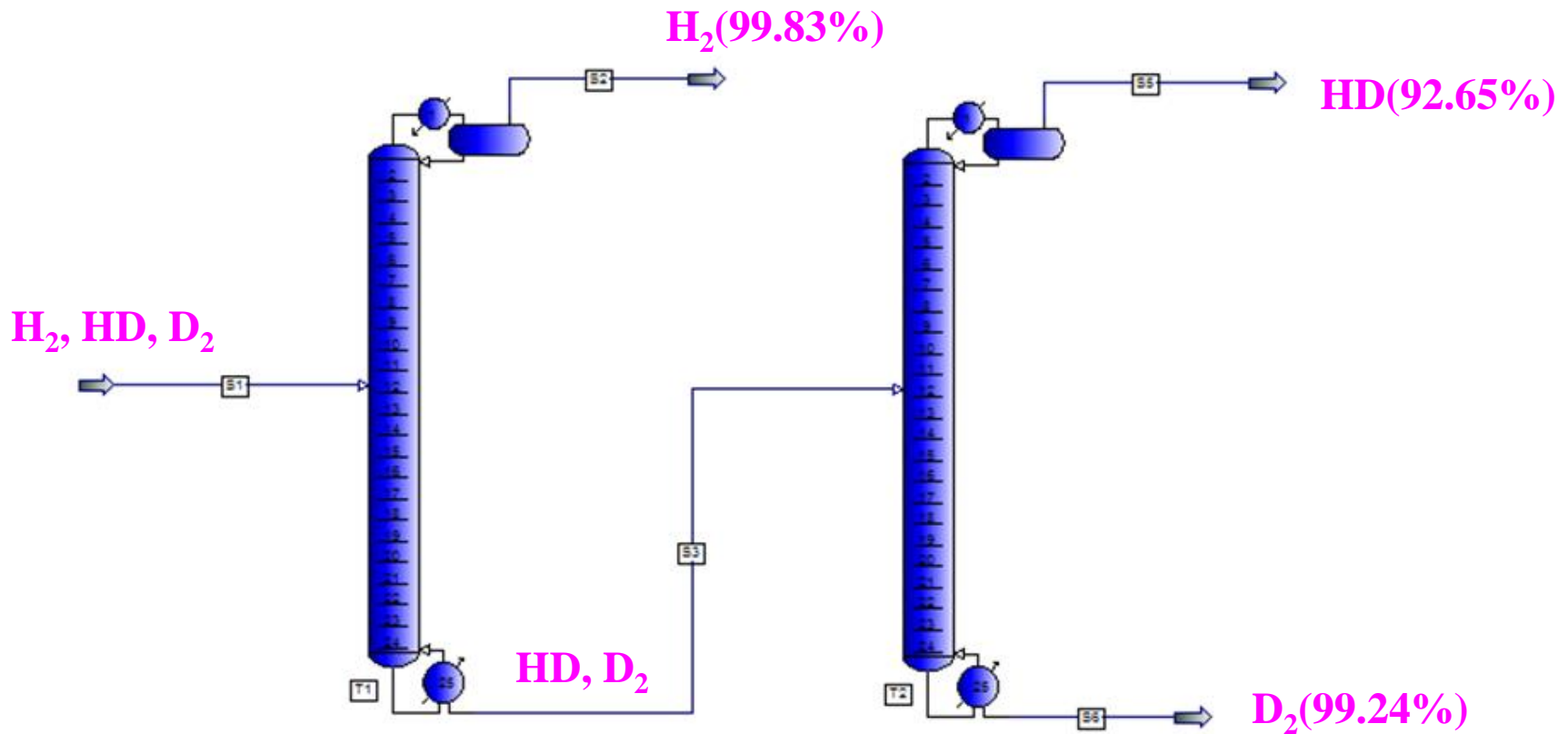
- Theoretical Stages: 25
- Condenser Outlet Pressure: 50 kPa
- Column Top Pressure: 55 kPa
- Column Pressure Drop: 5 kPa
- Feed Stage: 12

➤ 2nd Column

- Theoretical Stages: 25
- Condenser Outlet Pressure: 50 kPa
- Column Top Pressure: 55 kPa
- Column Pressure Drop: 5 kPa
- Feed Stage: 12

5. ITER ISS 공정 시뮬레이션 Case 1

[수소 동위원소 심냉 분리를 위한 전산모사 수행_전산모사]



Distillation Column Configuration with PRO/II.

5. ITER ISS 공정 시뮬레이션 Case 1

STREAM ID	S1	<u>S2</u>	S3	<u>S4</u>
NAME				
PHASE	VAPOR	VAPOR	LIQUID	VAPOR
THERMO ID	SRK01	SRK01	SRK01	SRK01
FLUID MOLAR FRACTIONS				
1 H2	0.3000	<u>0.9983</u>	0.0284	0.0640
2 HD	0.3000	1.7223E-03	0.4160	<u>0.9265</u>
3 D2	0.4000	4.7393E-06	0.5556	9.5268E-03
TOTAL RATE, KG-MOL/HR	10.0000	2.8000	7.2000	3.2000
TEMPERATURE, K	30.0000	18.5123	21.3201	20.1292
PRESSURE, KPA	120.0000	50.0000	60.0000	50.0000
ENTHALPY, M*KJ/HR	-0.0410	-0.0214	-0.0311	-0.0219
MOLECULAR WEIGHT	3.1246	2.0176	3.5551	2.9689
MOLE FRAC VAPOR	1.0000	1.0000	0.0000	1.0000
MOLE FRAC LIQUID	0.0000	0.0000	1.0000	0.0000

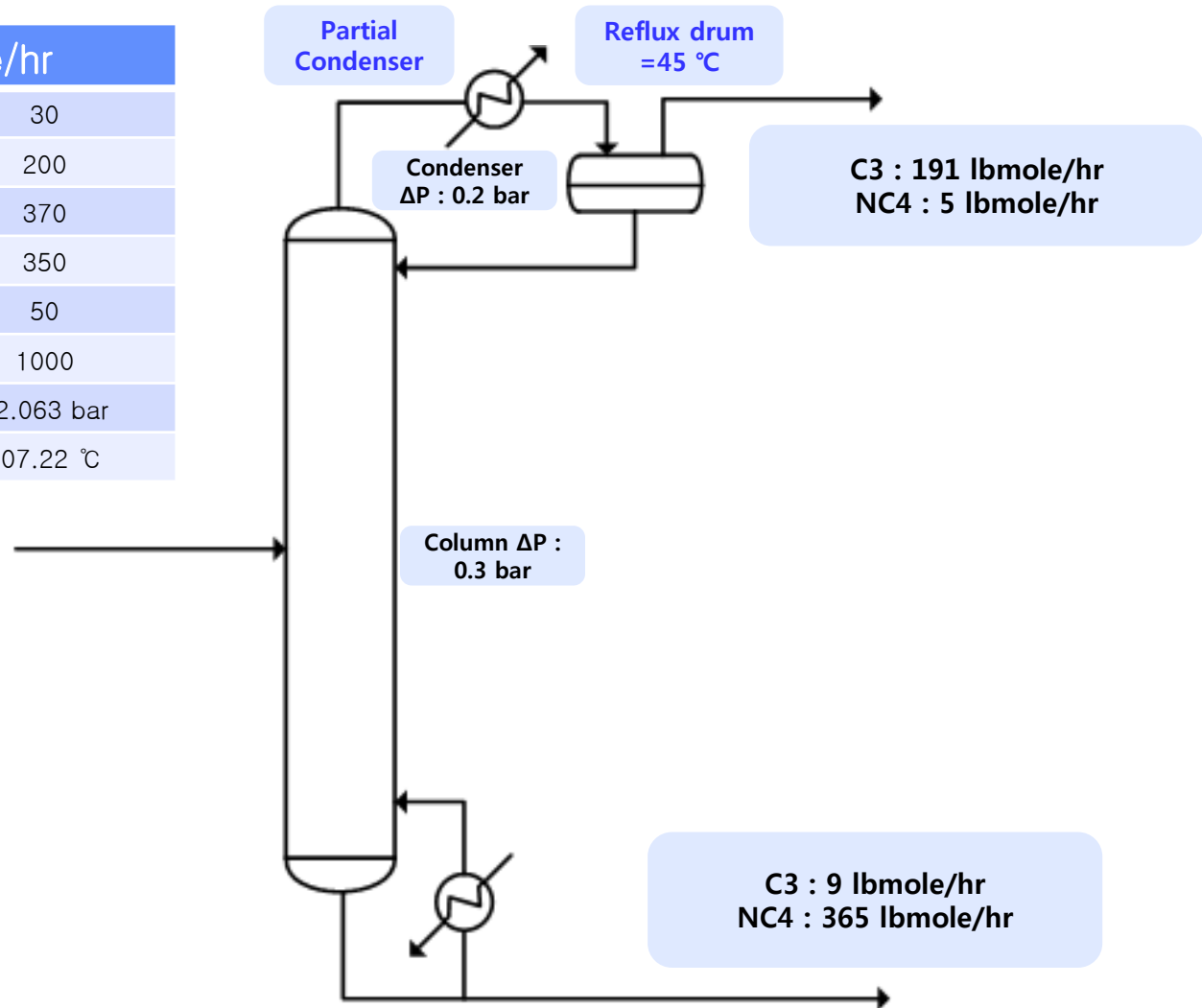
5. ITER ISS 공정 시뮬레이션 Case 1

STREAM ID	<u>S5</u>
NAME	
PHASE	LIQUID
THERMO ID	SRK01
FLUID MOLAR FRACTIONS	
1 H2	6.3811E-08
2 HD	7.6255E-03
3 D2	<u>0.9924</u>
TOTAL RATE, KG-MOL/HR	4.0000
TEMPERATURE, K	22.1247
PRESSURE, KPA	60.0000
ENTHALPY, M*KJ/HR	-5.5928E-03
MOLECULAR WEIGHT	4.0241
MOLE FRAC VAPOR	0.0000
MOLE FRAC LIQUID	1.0000

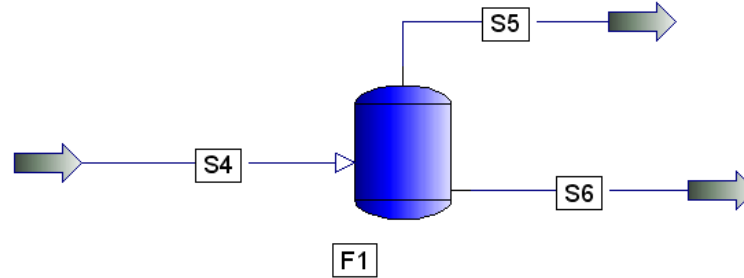
부록 : PRO/II를 활용한 증류탑 모사 방법

Feedstock characterization & product specifications

Feed, lbmole/hr	
C2	30
C3	200
NC4	370
NC5	350
NC6	50
Total	1000
Press.	22.063 bar
Temp.	107.22 °C



Column의 운전압력 결정: Flash drum 이용



Stream Name		S4	S5	S6
Stream Description				
Phase		Vapor	Vapor	Liquid
Temperature	C	107.2200	45.0000	45.0000
Pressure	BAR	22.0630	16.5401	16.5401
Enthalpy	M*KCAL/HR	0.5672	0.4397	n/a
Molecular Weight		42.5449	42.5449	44.0930
Mole Fraction Vapor		1.0000	1.0000	0.0000
Mole Fraction Liquid		0.0000	0.0000	1.0000
Rate	LB-MOL/HR	226.000	226.000	0.000
Fluid Rates	LB-MOL/HR			
C2		30.0000	30.0000	0.0000
C3		191.0000	191.0000	0.0000
NC4		5.0000	5.0000	0.0000
NC5		0.0000	0.0000	0.0000
NC6		0.0000	0.0000	0.0000

Column operating pressure : $16.54 + 0.2$ (Condenser ΔP) = **16.74 bar**

Column의 운전압력 결정: 탑상류 조성 추산치

PRO/II - Stream Data

UOM Range Help Tag Overview Status Notes

Stream: S1 Description:

To Unit: SCD1

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Flowrate and Composition...

Stream Solids Data...

Stream Polymer Data...

Thermal Condition

First Specification:

Temperature 107.22 C

Second Specification:

Pressure 22.063 bar

Thermodynamic System: Determined From Connectivity

OK Cancel

Push to bring up the flowrate and assay window

Stream Data - Flowrate and Composition

UOM Range Help Tag

Specify flowrate and composition for stream S4

Fluid Flowrate Specification

Total Fluid Flowrate: lb-mol/hr Total LV or GV rate on an Adjusted Standard Basis

Individual Component Flowrates

Copy	Component	Component Flowrate
Paste		lb-mol/hr
	C2	30.000
	C3	191.00
	NC4	5.0000
	NC5	
	NC6	

Clear Compositions Total: 226.00 Normalize Component Flowrates Based on Specified Fluid Flowrate

OK Cancel

Exit the window after saving all data

Column의 운전압력 결정: Partial condenser (Dew P)

PRO/II - Flash Drum

UOM Define Range Help Overview Status Notes

Unit: F1 Description:

First Specification

Temperature 45.00 C Thermodynamic System: Default (PR01)

Second Specification

Unit Specification: Dew Point
 Product Specification:
Parameter = value within the default tolerance

Temperature Estimate: C
Pressure Estimate: bar
Pseudostream Flowrate: 0.00000 lb-mol/hr
Phase Assignment: Default

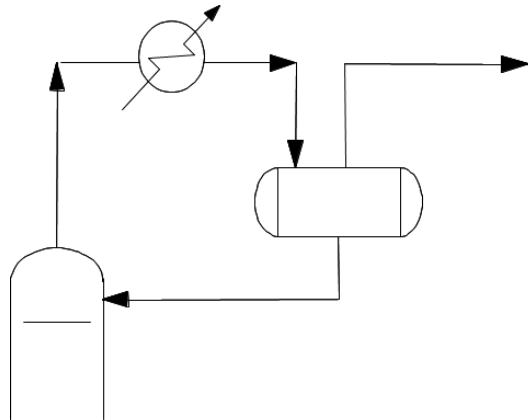
Product Phases...
Print Options...
Entrainment...

OK Cancel

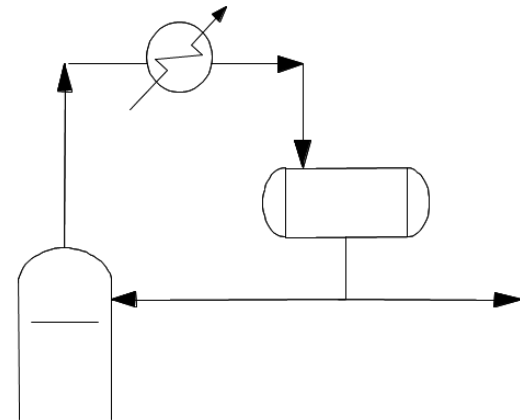
Exit the window after saving all data

Condenser type: 4가지 종류가 존재함

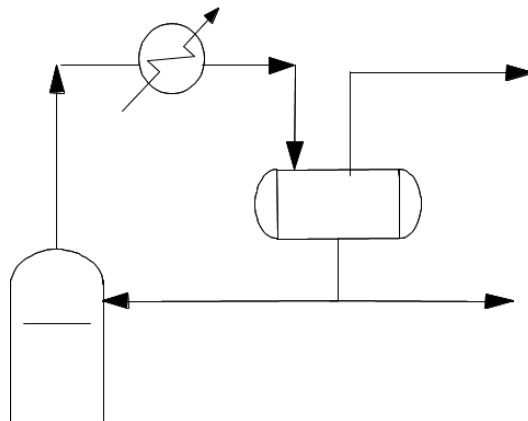
A. Partial



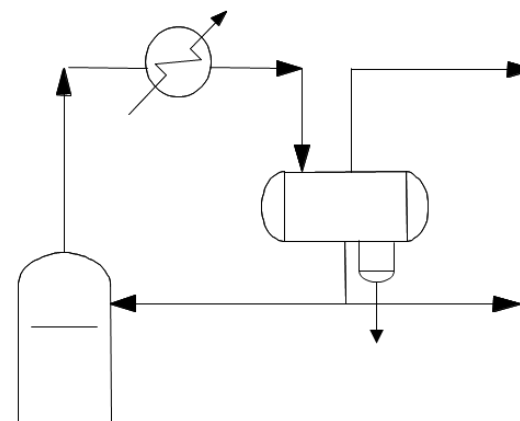
B. Bubble or sub-cooled



C. Mixed



D. Mixed with decanter



Shortcut Modeling

Shortcut Modeling: Feed 조건 입력

PRO/II - Stream Data

Stream: S1 Description:
To Unit: SCD1

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Flowrate and Composition...
Stream Solids Data...
Stream Polymer Data...

Thermal Condition

First Specification: Temperature 107.22 C
Second Specification: Pressure 22.063 bar

Thermodynamic System: Default (PR01)

Exit the window after saving all data

Stream Data - Flowrate and Composition

UDM Range Help Tag

Specify flowrate and composition for stream S1

Fluid Flowrate Specification

- Total Fluid Flowrate: 1000.0 lb-mol/hr
- Individual Component Flowrates
- Component Concentrations

Total Fluid Flowrate: lb-mol/hr

Total LV or GV rate on an Adjusted Standard Basis

Component	Composition Mole
C2	30.000
C3	200.00
NC4	370.00
NC5	350.00
NC6	50.000

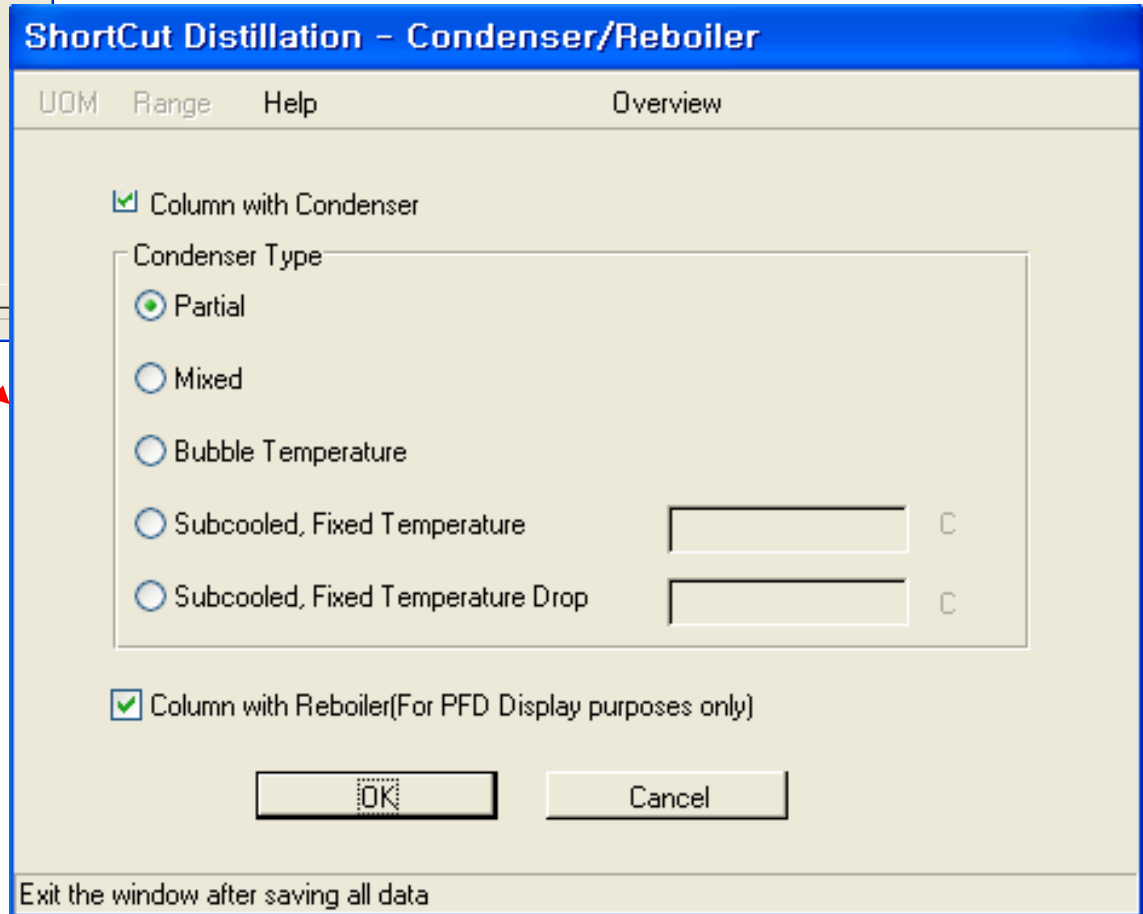
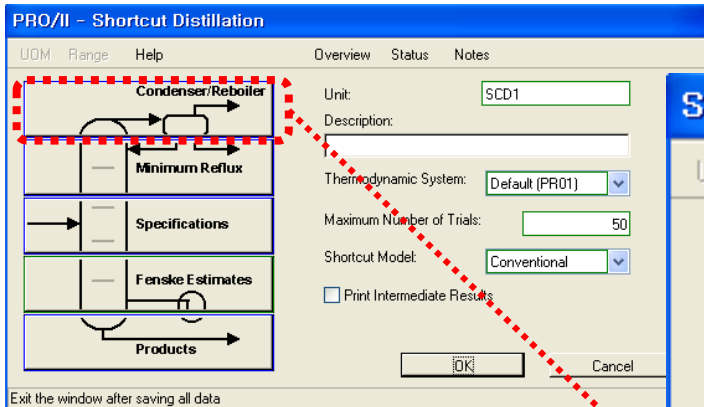
Clear Compositions Total: 1000.0

Normalize Component Flowrates Based on Specified Fluid Flowrate

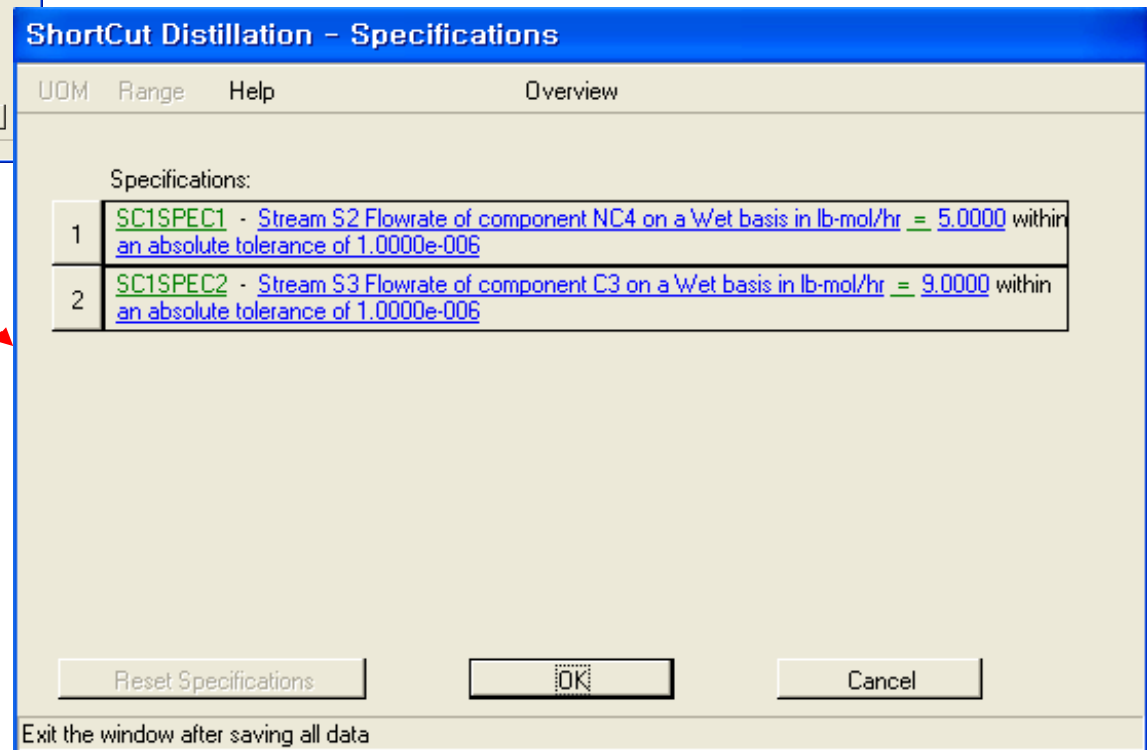
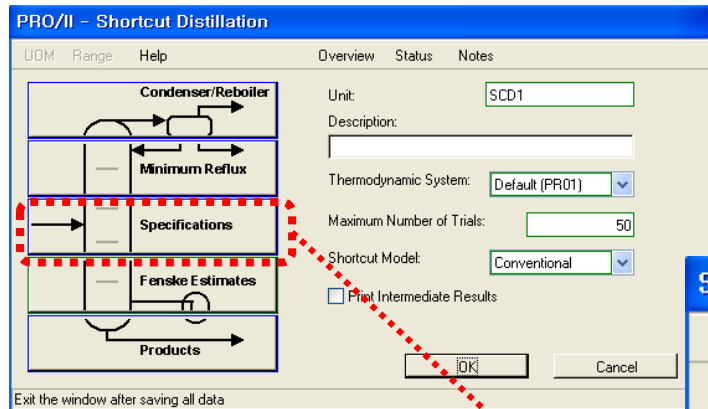
OK Cancel

Exit the window after saving all data

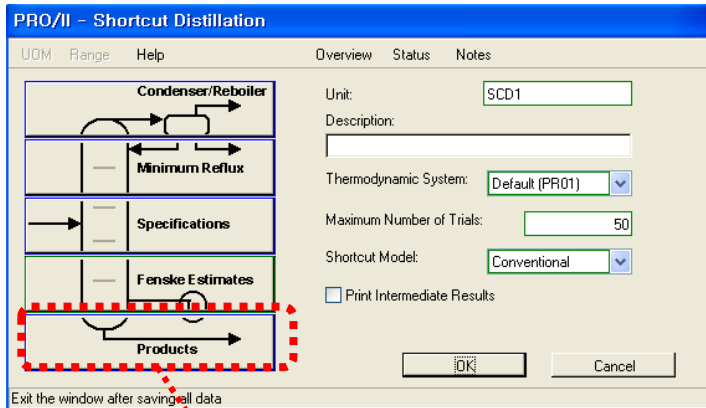
Shortcut Modeling: Partial condenser



Shortcut Modeling: Product specifications



Shortcut Modeling: Condenser pressure & ΔP



Top pressure & condenser, column pressure drop 입력

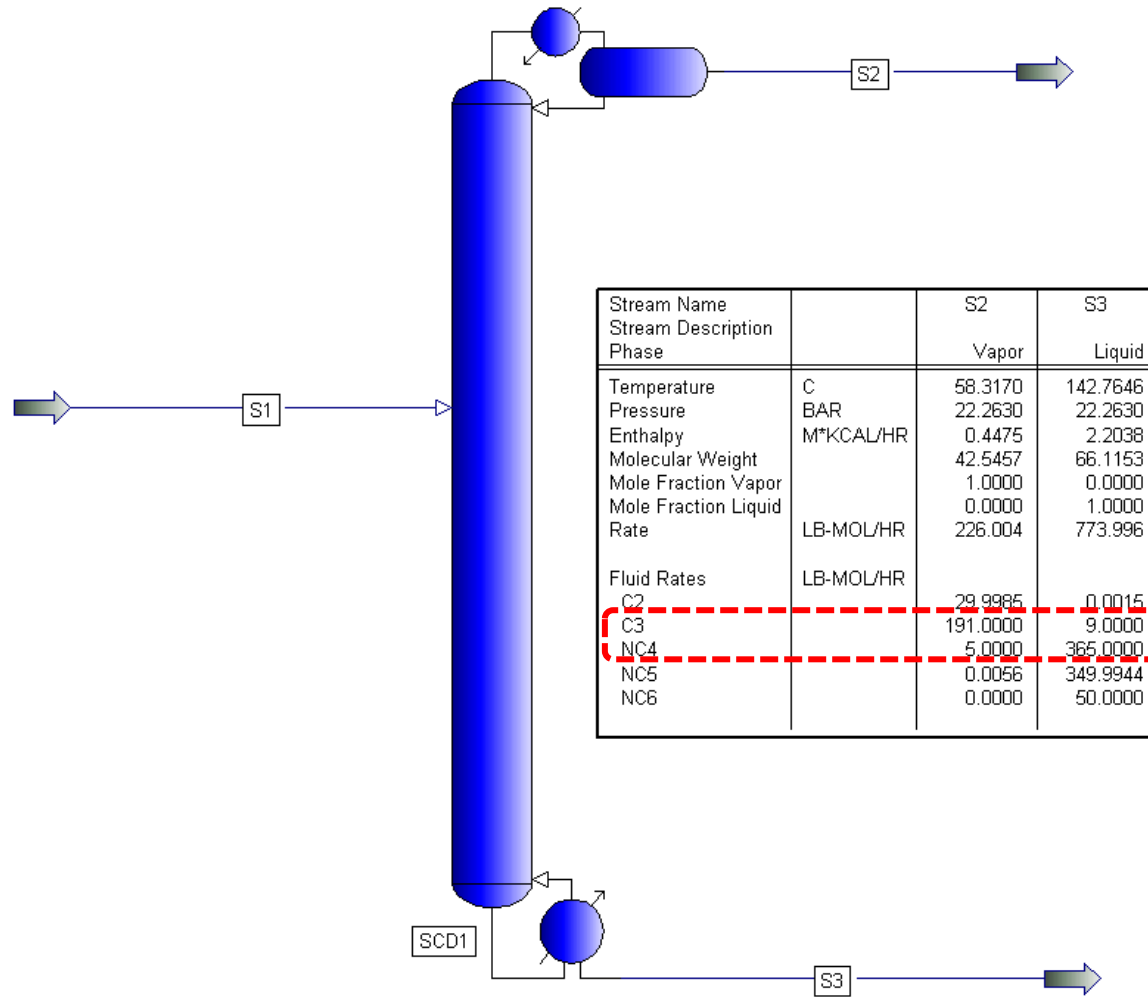
Shortcut Distillation - Products

	Product	Est. Type	Estimate	UOM	Phase	Pres. Type	Pressure	UQM
1	S2	Rate	500.00	lb-mol/hr	Vapor	Pressure	16.540	bar
2	S3			lb-mol/hr	Liquid	Delta P	0.50000	bar

Move Up Move Down OK Cancel

Exit the window after saving all data

Shortcut Modeling 결과



최소이론단수와 최소환류비

		TOTAL STREAM RATES					
STREAM + PHASE		MOLES LB-MOL/HR	WEIGHT LB/HR	LIQUID VOL M3/HR	NORM VAPOR (1) M3/HR	SECTION	NUM TRAYS
S2	V	226.00	9615.50	8.93	2297.74	1	12.85
S3	L	774.00	51173.01	37.91	7869.07		
TOTALS		1000.00	60788.51	46.85	10166.81		12.85

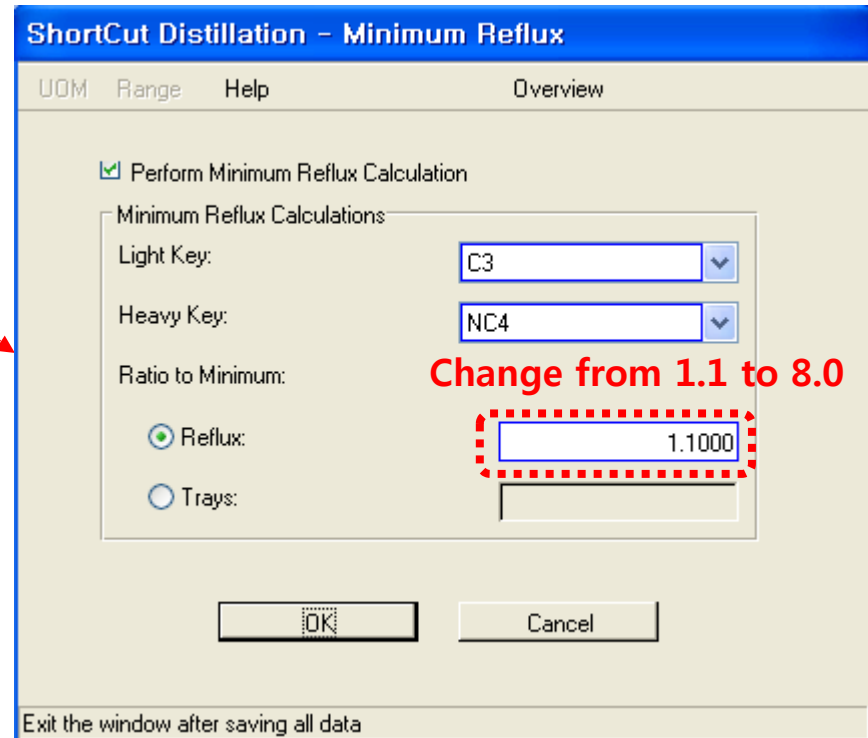
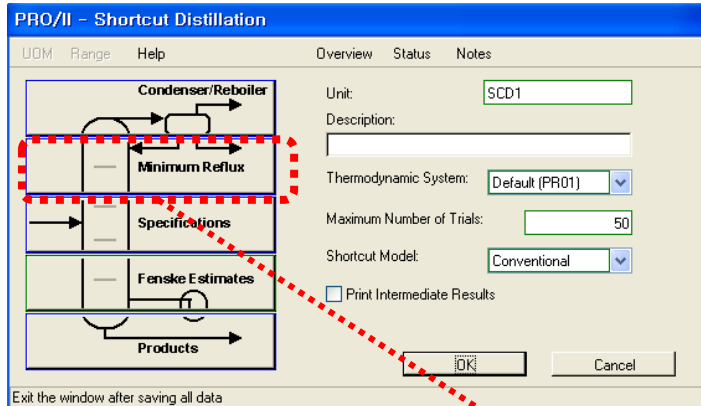
SPECIFICATIONS

PARAMETER TYPE	COMP. NUM	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
STRM S2	3	MOL RATE	5.000E+00	5.000E+00
STRM S3	2	MOL RATE	9.000E+00	9.000E+00

SUMMARY OF UNDERWOOD CALCULATIONS

MINIMUM REFLUX RATIO	3.22726
FEED CONDITION Q	1.07124
FENSKE MINIMUM TRAYS	12.84930
OPERATING REFLUX RATIO	10.00 * R-MINIMUM

Shortcut Modeling: Case study



최적이론단수와 최적환류비 결정

R/R-MIN	M/M-MIN	R	M	Total duty
1.050	2.756	3.389	35.413	2.6856
1.075	2.466	3.469	31.686	2.7327
1.100	2.378	3.550	30.556	2.7790
1.125	2.299	3.631	29.541	2.8250
1.150	2.228	3.711	28.628	2.8710
1.225	2.048	3.953	26.315	3.0090
1.300	1.908	4.195	24.516	3.1490
1.375	1.796	4.437	23.077	3.2870
1.450	1.709	4.680	21.959	3.4250
1.500	1.675	4.841	21.523	3.5180
1.625	1.602	5.244	20.585	3.7490
1.750	1.542	5.648	19.814	3.9800
1.800	1.522	5.809	19.557	4.0730
2.000	1.452	6.455	18.657	4.4430
2.200	1.398	7.100	17.963	4.8110
2.500	1.336	8.068	17.167	5.3670
2.875	1.280	9.278	16.447	6.0590
3.250	1.243	10.489	15.972	6.7530
3.500	1.224	11.295	15.728	7.2150
4.125	1.187	13.312	15.252	8.3710
4.750	1.160	15.329	14.905	9.5250
5.000	1.152	16.136	14.802	9.9870
6.000	1.125	19.364	14.455	11.8370
7.000	1.106	22.591	14.211	13.6850
8.000	1.092	25.818	14.031	15.5330
9.750	1.075	31.466	13.813	18.7690
11.500	1.063	37.113	13.659	22.0000

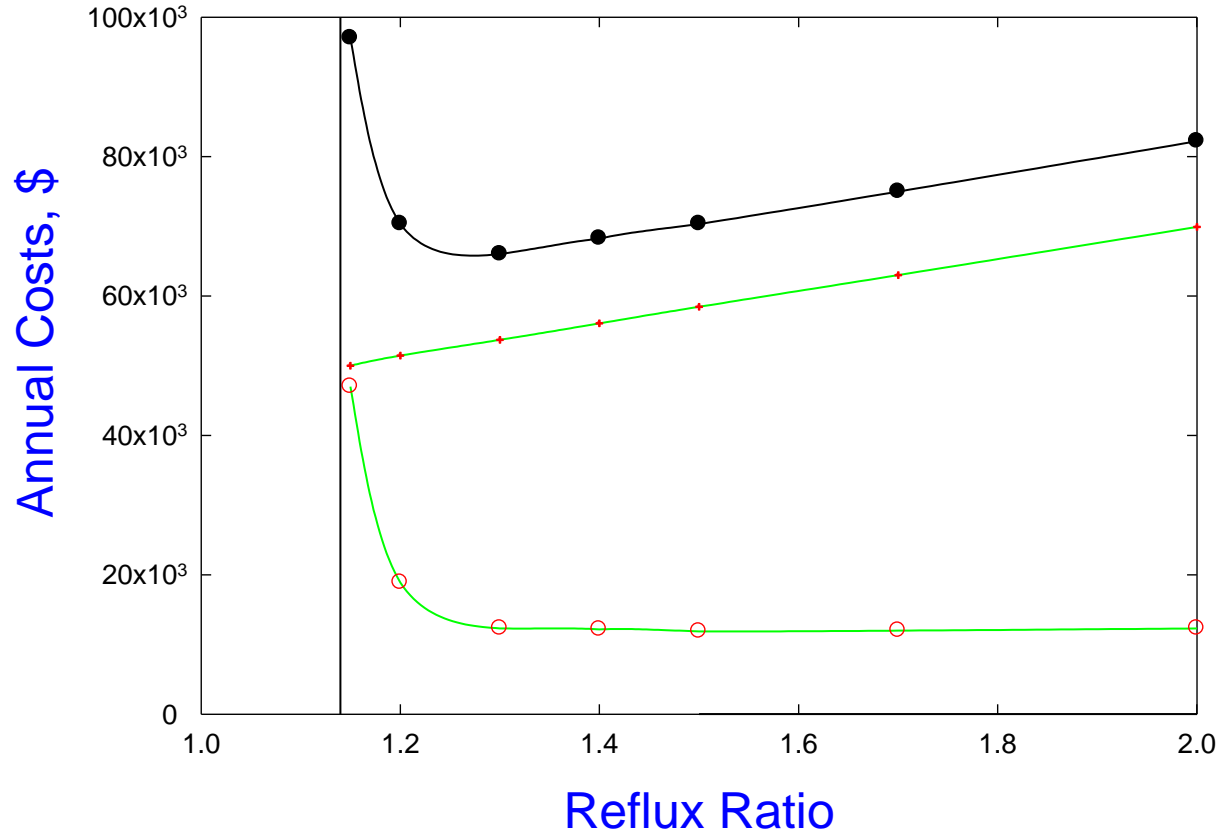
$R/R-MIN * R-MIN = R$
 $R-MIN : 3.22726$

$M/M-MIN * M-MIN = M$
 $M-MIN : 12.84930$

ABS(Condenser duty)
 +
 ABS(Reboiler duty)

Example: 환류비에 따른 연간 비용

벤젠-톨루엔 증류의 경우



Rigorous modeling

Depropanizer column: Feedstock characterization

PRO/II - Stream Data

UOM Range Help Tag Overview Status Notes

Stream: S1 Description:

To Unit: SCD1

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Flowrate and Composition...

Stream Solids Data...

Stream Polymer Data...

Thermal Condition

First Specification:

Temperature 107.22 C

Second Specification:

Pressure 22.063 bar

Thermodynamic System: Determined From Connectivity

OK Cancel

Push to bring up the flowrate and assay window

Stream Data - Flowrate and Composition

UOM Range Help Tag

Specify flowrate and composition for stream S1

Fluid Flowrate Specification

Total Fluid Flowrate: 1000.0 lb-mol/hr Total LV or GV rate on an Adjusted Standard Basis

Individual Component Flowrates

Copy	Component	Composition Mole
Paste	C2	30.000
	C3	200.00
	NC4	370.00
	NC5	350.00
	NC6	50.000

Clear Compositions Total: 1000.0 Normalize Component Flowrates Based on Specified Fluid Flowrate

OK Cancel

Exit the window after saving all data

Depropanizer column: Pressure profile

PRO/II - Column

UOM Range Help Overview Status Notes

Pressure Profile...
Feeds and Products...
Convergence Data...
Thermo-dynamic Systems...
Reboiler...

Tray Hydraulic/Packing...
Tray Efficiencies...

Condenser...
Heaters and Coolers...
Initial Estimates...
Pumparounds...
Performance Specifications

Unit: T1
Description:
Number of Stages: 17
Number of Iterations: 15
Algorithm: Inside-Out
Calculated Phases: Vapor-Liquid

Reactions...
Print
OK

Push to bring up the pressure profile window

Column - Pressure Profile

UOM Define Range Help Overview

Pressure Specification Mode

Overall
 By Individual Trays

Overall Specification

Top Tray Pressure: 16.540 bar

Pressure Drop

Per Tray: 0.00000 bar
 Column: 0.30000 bar

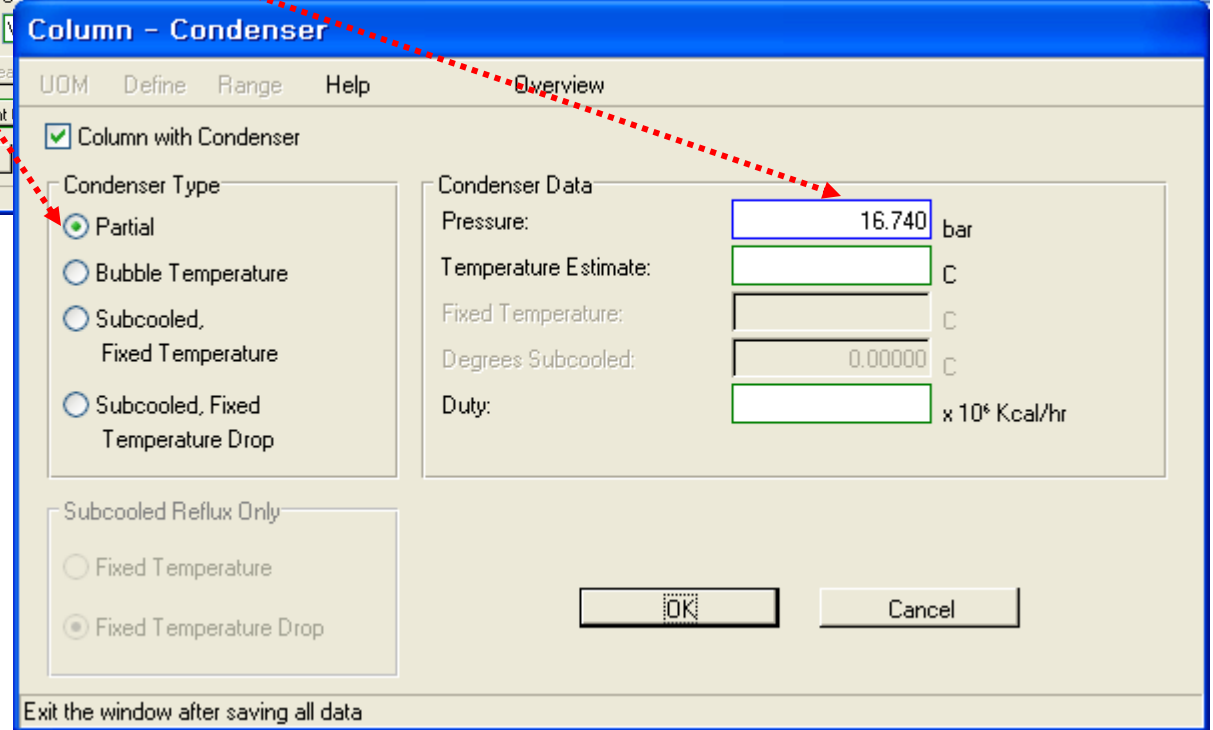
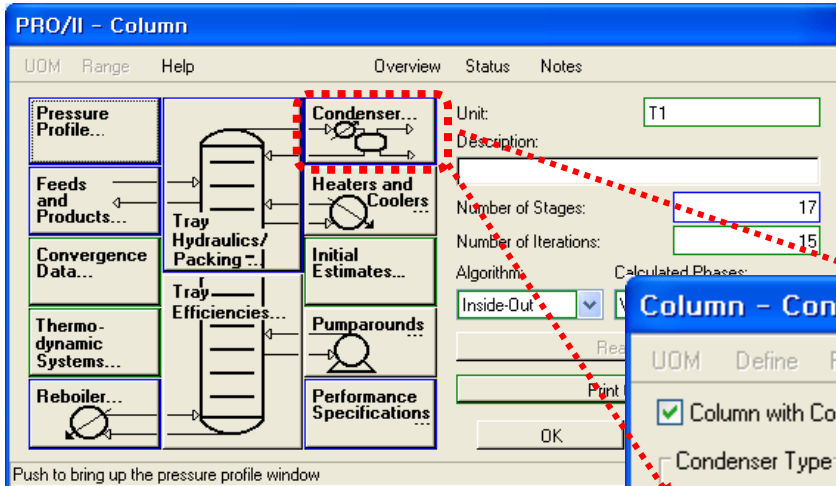
Individual Tray Specification

	Tray	Pressure bar
Cut		
Copy		
Paste	1	1
Insert	2	17
Reset	3	
	4	
	5	

OK Cancel

Exit the window after saving all data

Depropanizer column: Condenser type & pressure



Depropanizer column: Product specifications

PRO/II - Column

UOM Range Help Overview Status Notes

Pressure Profile... Feeds and Products... Convergence Data... Thermo-dynamic Systems... Reboiler...

Tray Hydraulics/Packing... Tray Efficiencies...

Condenser... Heaters and Coolers... Initial Estimates... Pumparounds... Performance Specifications

Unit: Description: Number of Stages: Number of Iterations: Algorithm: Inside-Out

Exit the window after saving all data

Column - Specifications and Variables

UOM Range Help Overview

Add Specifications and Variables

Specifications:

	Specifications:	Active:
1	COL1SPEC1 - Stream S8 Flowrate of component NC4 on a Wet basis in lb-mol/hr = 5.0000 within an absolute tolerance of 1.0000e-006	<input checked="" type="checkbox"/>
2	COL1SPEC2 - Stream S9 Flowrate of component C3 on a Wet basis in lb-mol/hr = 9.0000 within an absolute tolerance of 1.0000e-006	<input checked="" type="checkbox"/>

Variables:

1	Column T1 Duty of Heater CONDENSER
2	Column T1 Duty of Heater REBOILER

The number of active specifications, 2 equals the number of Variables, 2

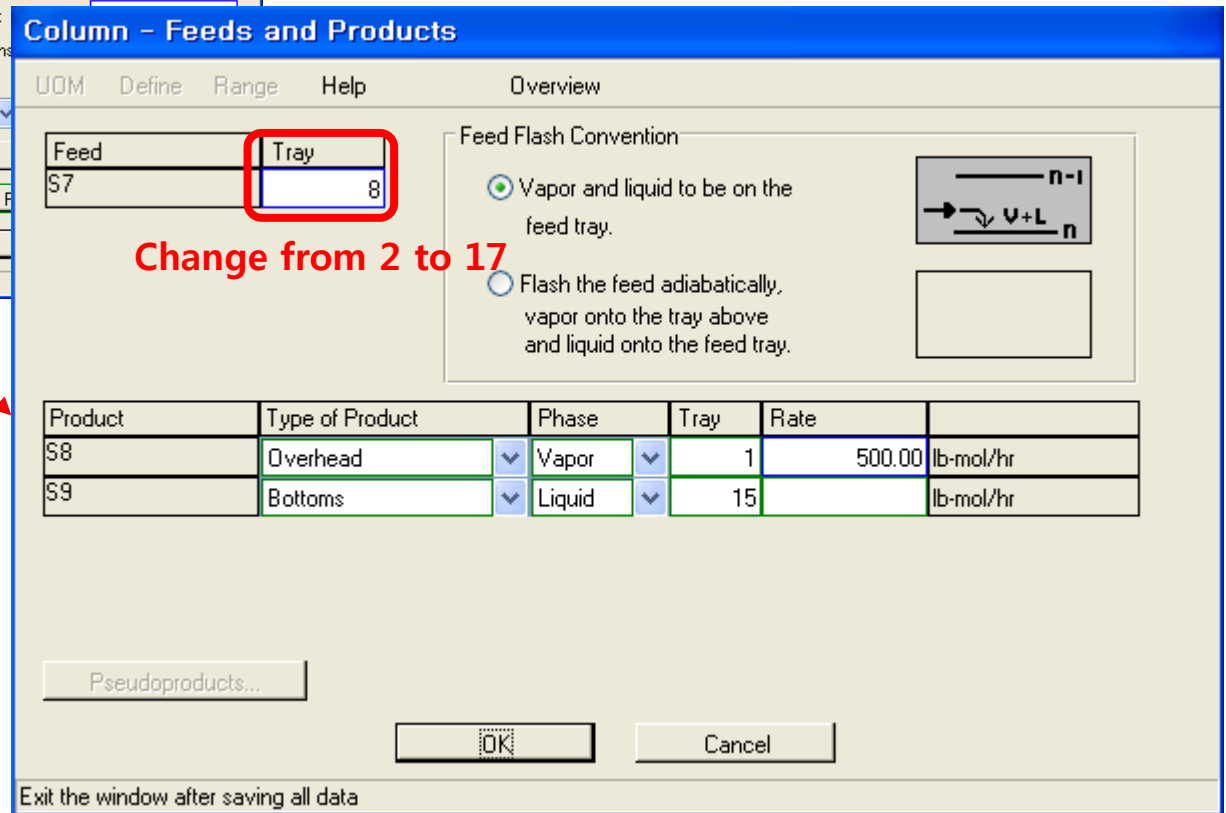
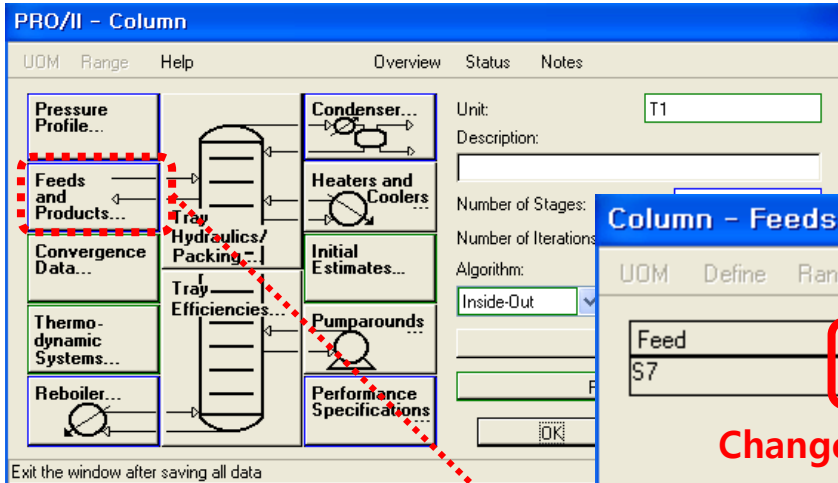
Data changes in this window will reinitialize column estimates

Insert Specification/Variable Insert Inactive Specification OK

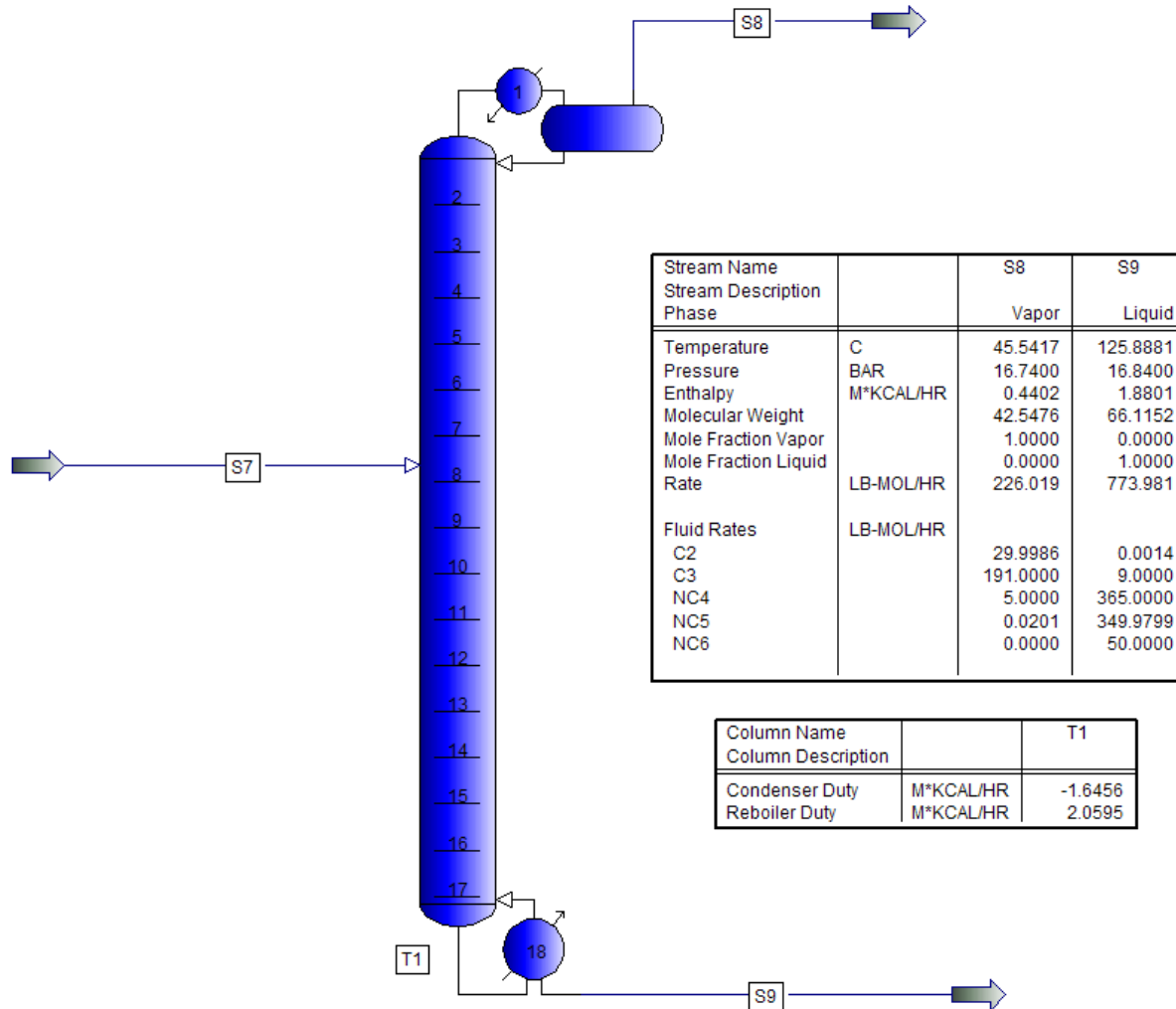
Cut Specifications/Variables Reset Specifications/Variables Cancel

Exit the window after saving all data

최적의 원료 주입단의 결정

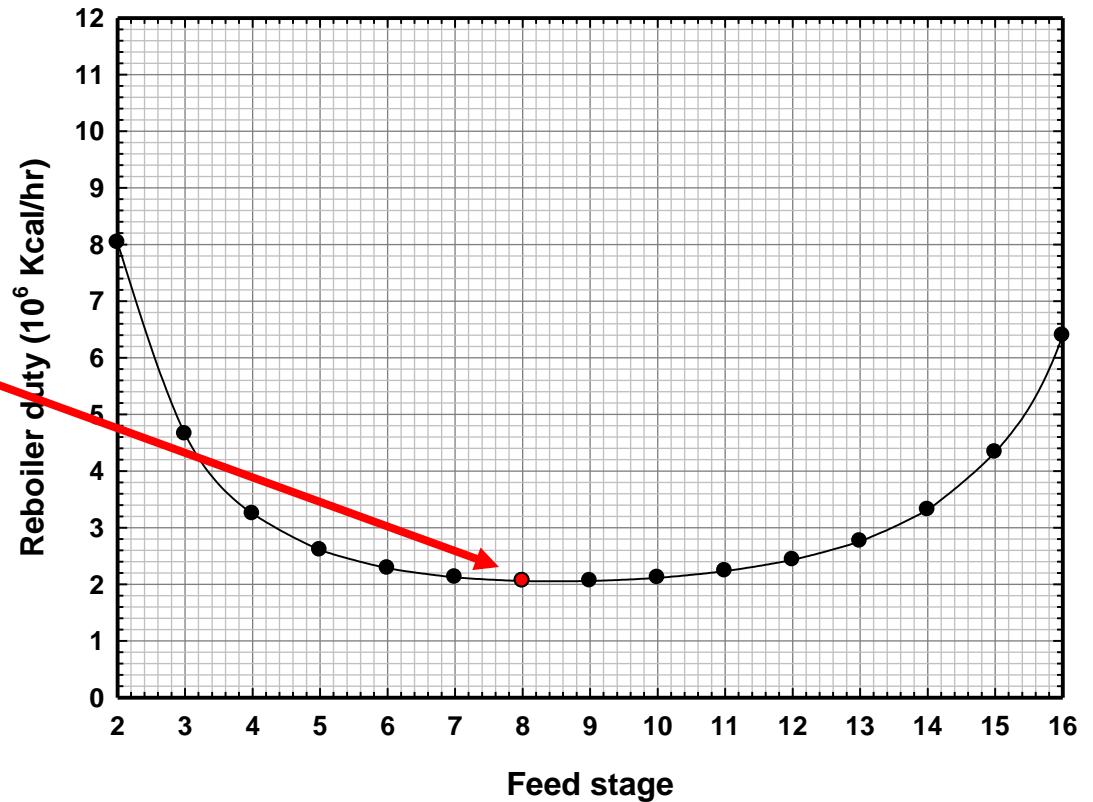


Depropanizer column: Rigorous modeling



최적의 원료 주입 단의 위치 결정

Feed tray	Reboiler duty (10^6 Kcal/hr)
2	8.0338
3	4.6530
4	3.2443
5	2.6027
6	2.2828
7	2.1229
8	2.0577
9	2.0586
10	2.1138
11	2.2325
12	2.4316
13	2.7582
14	3.3128
15	4.3301
16	6.3894
17	11.0385



Column의 Tray Sizing

PRO/II - Column

UOM Range Help Overview Status Notes

Pressure Profile... Feeds and Products... Convergence Data... Thermo-dynamic Systems... Reboiler...

Tray Hydraulics/Packing... Tray Efficiencies... Condenser... Heaters and Coolers... Initial Estimates... Pumparounds... Performance Specifications...

Unit: T1
 Description:
 Number of Stages:
 Number of Reactions:
 Algorithm: Inside-Out Vapor-Liquid
 Reactions...
 Print Options...
 OK Cancel

Push to bring up the tray hydraulics window

Column - Tray Hydraulics

UOM Range Help Overview

Cut	Section Name	Starting Tray	Ending Tray	Internals	Calculation Type	Calculation Data
Reset	1 COLSECT-1	2	7	Trays	Sizing	Enter Data...
	2 COLSECT-2	8	16	Trays	Sizing	Enter Data...
	3					Enter Data...
	4					Enter Data...
	5					Enter Data...

OK Cancel

Push to bring up the rating/sizing window

Column - Tray Sizing

UOM Range Help

Tray Type: VALVE

Minimum Tray Diameter: 381.00 mm

Tray Spacing: 609.60 mm

Flooding Factor: 85.00 %

System Loading Factor: 1.00

Number of Flow Paths: Calculated

Estimated Diameter: mm

Weir Height: mm

OK Cancel

Exit the window after saving all data

Perform Tray Sizing Calculations

- At output time
- During column convergence and do not update pressure profile
- During column convergence and update the pressure profile

Calculated pressure drop will be based on number of trays divided by a scaling factor of 1.0

Column의 Tray Sizing: 결과

TRAY SIZING DOWNCOMER WIDTH CALCULATION

TRAY	NEXT LARGER	DOWNCOMER WIDTHS		
	DIAMETER MM	SIDE MM	CENTER MM	OFF-CENTER MM
2	1219.	256.093	N/A	N/A
3	1219.	255.781	N/A	N/A
4	1219.	255.528	N/A	N/A
5	1219.	255.667	N/A	N/A
6	1219.	255.852	N/A	N/A
7	1219.	255.871	N/A	N/A
8	1372.	370.158	N/A	N/A
9	1372.	381.453	N/A	N/A
10	1372.	379.738	N/A	N/A
11	1372.	378.371	N/A	N/A
12	1372.	377.110	N/A	N/A
13	1372.	376.030	N/A	N/A
14	1524.	415.111	N/A	N/A
15	1524.	414.112	N/A	N/A
16	1524.	413.386	N/A	N/A
17	1524.	413.054	N/A	N/A

SECTION	DESIGN	DIAMETER MM	NP	NUMBER	DOWNCOMER WIDTHS		
	TRAY NUMBER			OF VALVES OR CAPS	SIDE MM	CENTER MM	OFF-CENTER MM
COLSECT-1	2	1219.	1	104	256.093	N/A	N/A
COLSECT-2	14	1524.	1	131	415.111	N/A	N/A

감사합니다