ISS(Isotope Separation System)

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6. ITER ISS 공정 시뮬레이션 Case 2

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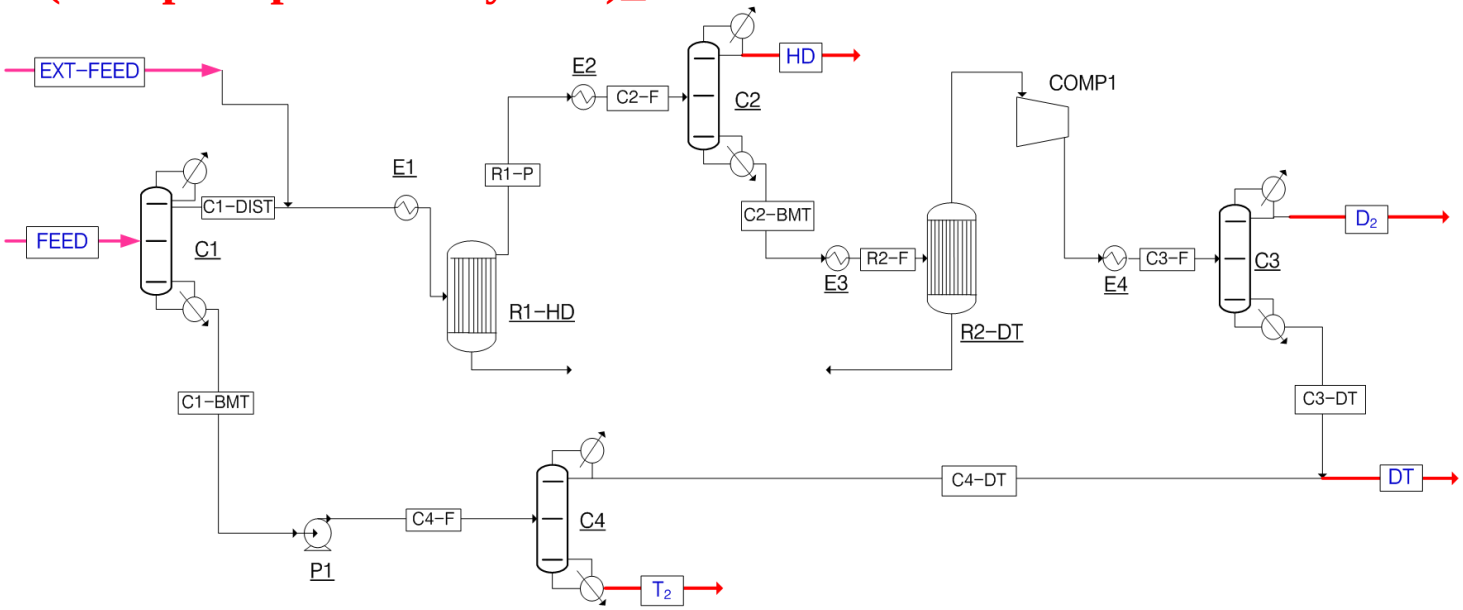

- ❖ 본 연구에서 다루는 ISS는 4기의 증류탑과 2기의 평형반응공정으로 이루어져 있음.
- ❖ 동위 원소체들을 초저온(20K 근처)에서 증류하기 위해서는 **헬륨냉매(15~ 18K 근처)를 이용한 냉동사이클이** 필요
- ❖ Aspen Tech사의 Aspen Plus내에 DB로 내장하고, 원하는 조성의 **D_2(99.00 mol% 이상), DT (98.00 mol% 이상), T_2 (94.00 mol% 이상)**를 생산하기 위한 초저온증류탑과 평형반응기 그리고 헬륨냉동사이클을 모델링.

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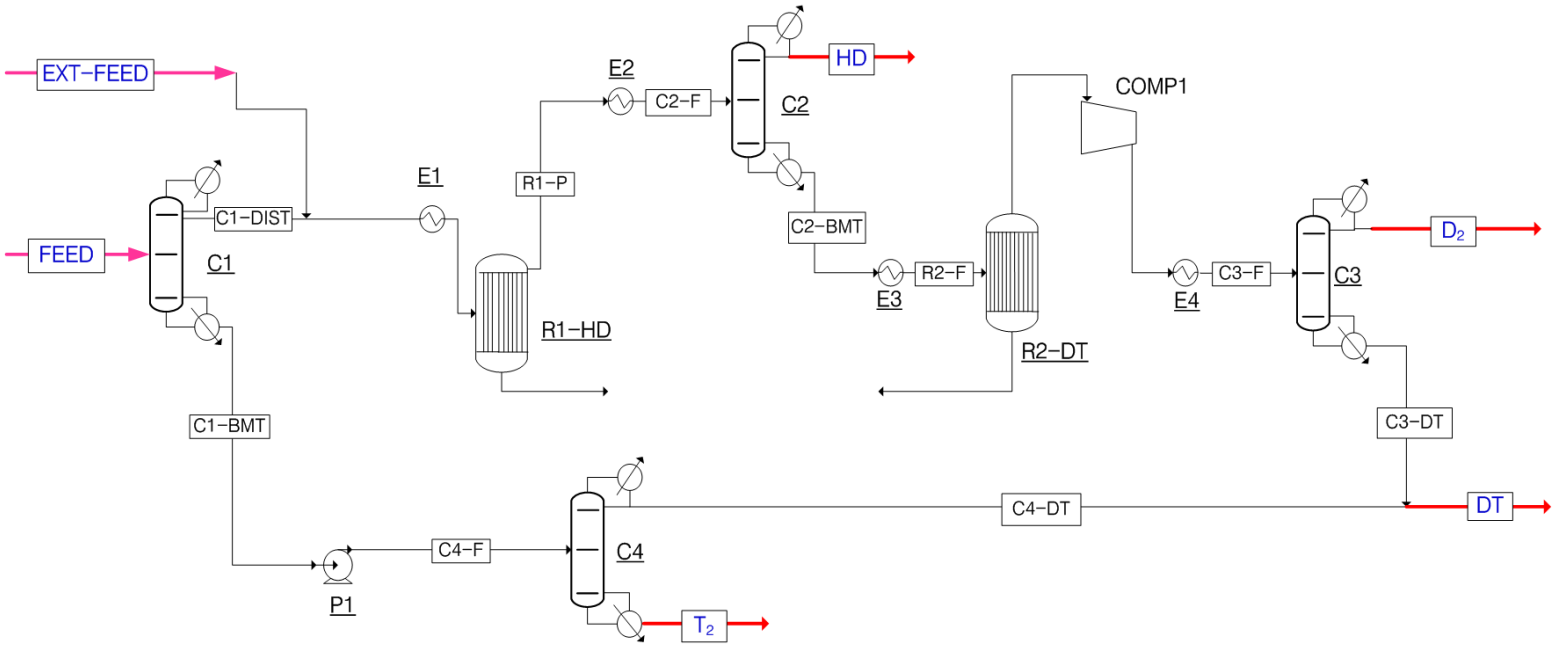
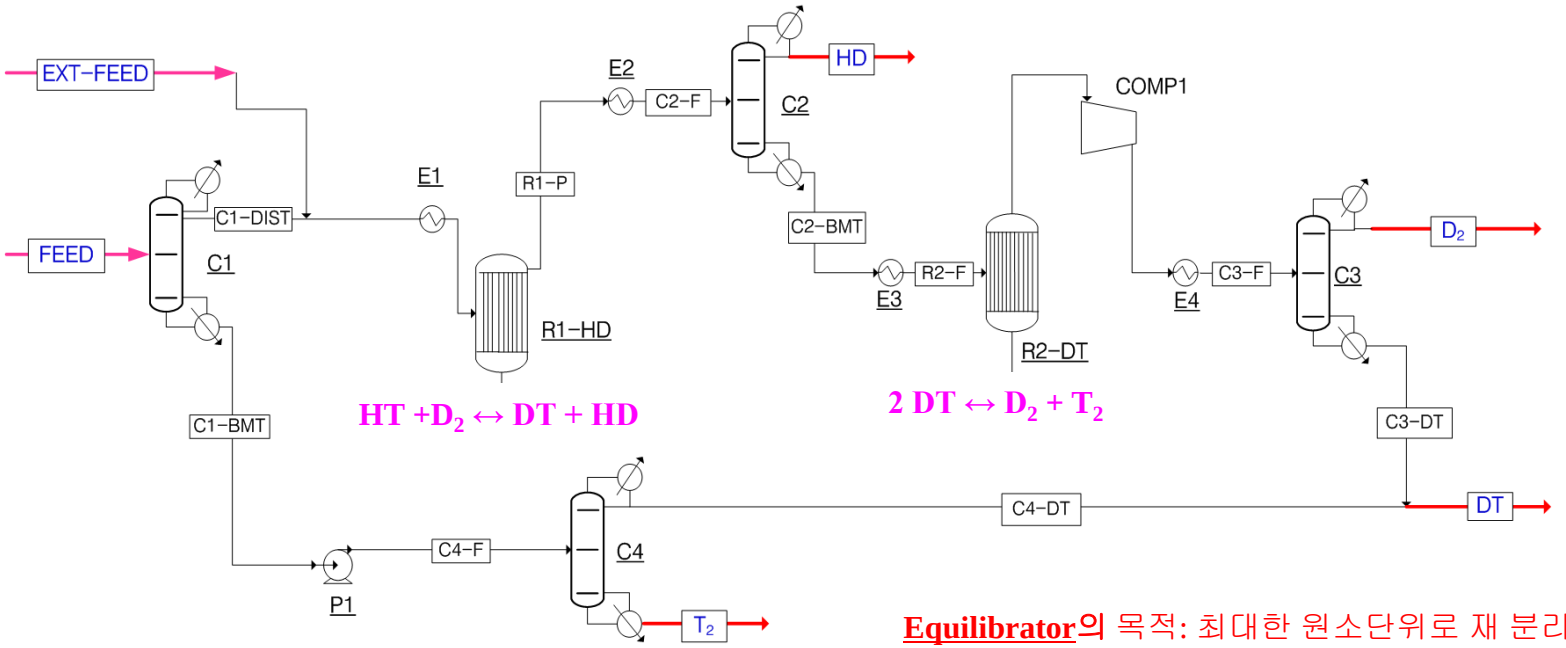


Stream number	C1	C2	C3	C4
Reflux ratio	54.75	82.06	13.25	56.55
Top distillate rate (gmole/h)	29.77	1,600.00	930.00	58.88
Number of stages	80.00	80.00	80.00	180.00
Feed stage	50.00	55.00	40.00	67.00
Column top press. (kPa)	91.19	70.93	81.06	106.39

6. ITER ISS 공정 시뮬레이션 Case 2



Equilibrator의 목적: 최대한 원소단위로 재 분리하는 역할

평형반응장치의 최적 배열과 위치가 존재

$D_2 + T_2$ <=> 2DT

Equilibrium constant : $K_{DT} = [DT]^2 / [D_2][T_2]$

Reaction rate : $R_{DT} = r_{DT}\, f(P_{DT}, P_{D2}, P_{T2})$

Reactions in the equilibrators

- $HT + D_2 \leftrightarrow DT + HD$
- $2\,DT \leftrightarrow D_2 + T_2$

equilibrium equation	온도(K)					
	0	273.1	298.1	400	500	600
$[HD]^2/[H_2][D_2]$	0	3.18	3.25	3.48	3.62	3.72
$[HT]^2/[H_2][T_2]$	0	2.42	2.56	2.97	3.24	3.44
$[DT]^2/[D_2][T_2]$	0	3.79	3.82	3.88	3.92	3.94

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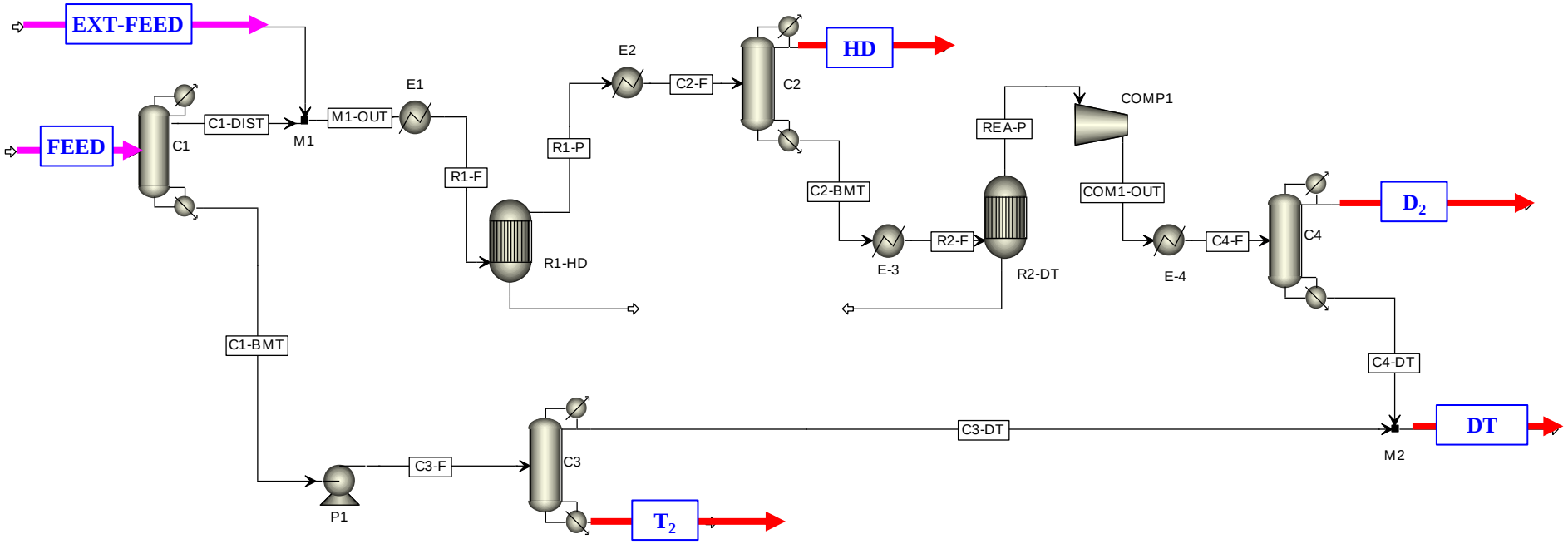

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- The Isotope Separation System (ISS) has been simulated using Aspen Plus steady-state simulators.
- This system has four distillation columns and two equilibrium reactors. This system has four purified products, HD, D_2, DT and T_2.

6. ITER ISS 공정 시뮬레이션 Case 2

➢ **Feedstock Information and Product Specifications**

Stream Name	FEED	EXT-FEED
Component	Mole%	
H_2	1.0	10.0
HD	0.0	5.0
D_2	24.0	80.0
DT	50.0	0.0
HT	0.0	5.0
T_2	25.0	0.0
Total	100.0	100.0
Temperature (K)	20.0	20.0
Pressure (ATM)	1.1	1.1
Flow (mol/min)	2.0	1.0

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- Design and operating conditions for each distillation columns are as:

Column Name	Column 1	Column 2	Column 3	Column 4
Reflux Ratio	25	150	8	8
Top Distillate Rate (mole/min)	0.5	0.3	1	1.75
Number of Stages	80	80	65	80
Feed Stage	50	55	30	40
Column Top Press. (atm)	0.9	0.7	1.04	0.8
Stage Pressure drop (atm)	0.02	0.003	0.0007	0.003

6. ITER ISS 공정 시뮬레이션 Case 2

- Design and operating conditions for Reactors

  - ✓ Chemical reactor operating temperature: 25^{o}C

  - ✓ When all hydrogen isotopes, i.e. H2, HD, HT, D2 and T2 are in equilibrium, there are following three equilibrium reactions are possible.

  - ✓ Their corresponding equilibrium constants at 298.15K are:

6. ITER ISS 공정 시뮬레이션 Case 2

- The role of Column 1 is to separate D_2 and DT.
  - **Design specification 1 and Variable 1:**
    - ✓ 99% recovery of D2 as a top distillate
    - ✓ Vary Distillate to feed ratio (0.001 to 1)
  - **Design specification 2 and Variable 2:**
    - ✓ 99.9% recovery of DT as a bottom product
    - ✓ Vary Reflux ratio (1 to 100)

	FEED	C1-DIST	C1-BMT
Temperature K	30	23.4433	24.23478
Pressure atm	1.1	0.9	0.92
Vapor Frac	1	0	0
Mole Flow kmol/hr	0.12	0.029773	0.090227
Mole Flow kmol/hr			
H2	0.0012	0.0012	9.56E-09
HD	0	0	0
HT	0	0	0
D2	**0.0288**	**0.02851**	0.000298
DT	**0.06**	6.00E-05	**0.05994**
T2	0.03	9.41E-07	0.029999

D2 recovery: 99% at top

DT recovery: 99.9% at bottom

6. ITER ISS 공정 시뮬레이션 Case 2

Column 1:

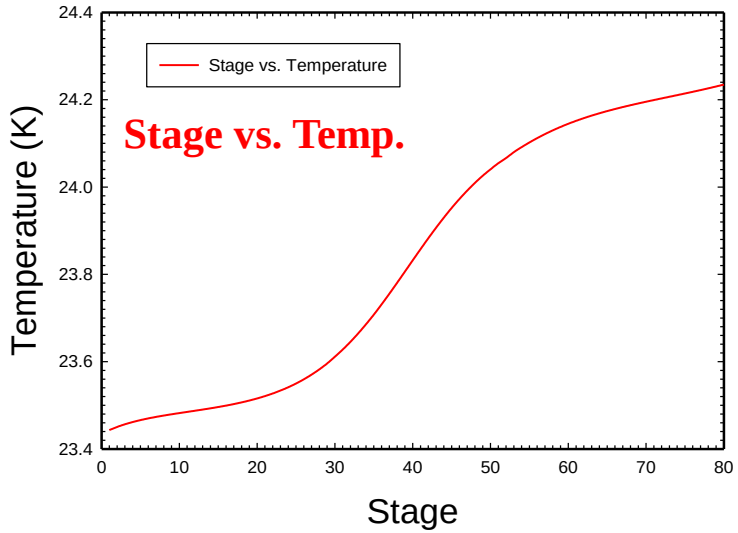
Column Name	Column 1
Reflux Ratio	54.75
Top Distillate Rate (mole/min)	0.5
Number of Stages	80
Feed Stage	50
Column Top Press. (atm)	0.9
Stage Pressure drop (atm)	0.02

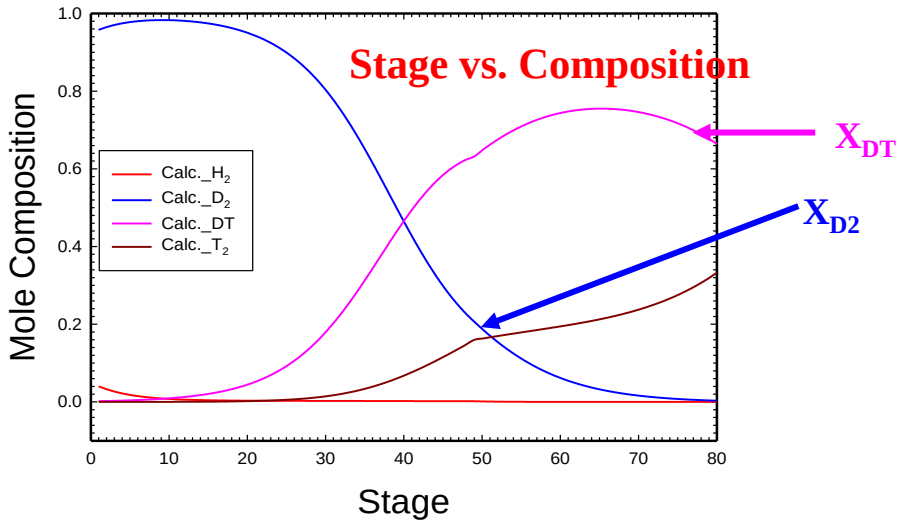
Result Summary

View: Condenser / Top stage Basis: Mole

Condenser / Top stage performance

Temperature:	23.4432987	K
Subcooled Temperature:		
Heat duty:	-0.6075241	kW
Subcooled duty:		
Distillate rate:	0.02977293	kmol/hr
Reflux rate:	1.63020267	kmol/hr
Reflux ratio:	54.7545222	
Free water distillate rate:		
Free water reflux ratio:		





6. ITER ISS 공정 시뮬레이션 Case 2

- The role of this Column 2 is to separate HT and D_2.
  - **Design specification 1 and Variable 1:**
    - ✓ 80% recovery of HT as a top distillate
    - ✓ Vary Distillate to feed ratio (0.001 to 1)
  - **Design specification 2 and Variable 2:**
    - ✓ 99% recovery of D_2 as a bottom product
    - ✓ Vary Reflux ratio (1 to 150)

	C2-F	HD	C2-BMT
Temperature K	20	21.44345	22.70514
Pressure atm	1	0.7	0.703
Mole Flow kmol/hr	0.089773	0.019474	0.070299
Mole Flow kmol/hr			
H2	0.001028	0.001025	2.13E-06
HD	0.015345	0.015345	4.03E-08
HT	**0.003**	**0.0024**	0.0006
D2	**0.07034**	0.000703	**0.06964**
DT	6.00E-05	5.66E-12	6.00E-05
T2	9.41E-07	3.37E-15	9.41E-07

HT recovery: 80% at top

D2 recovery: 99% at bottom

6. ITER ISS 공정 시뮬레이션 Case 2

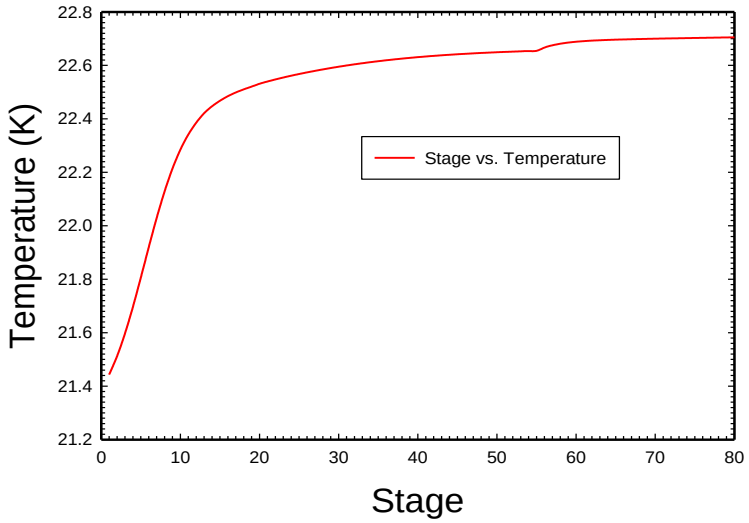
Column 2:

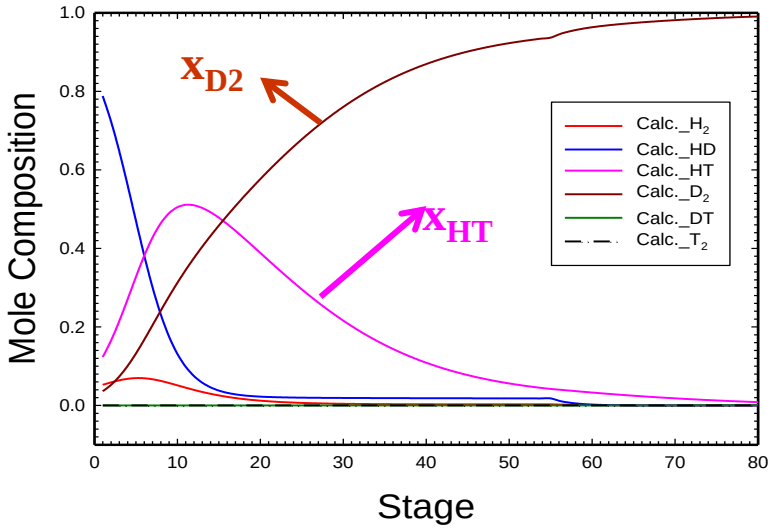
Column Name	Column 2
Reflux Ratio	82
Top Distillate Rate (mole/min)	0.3
Number of Stages	80
Feed Stage	55
Column Top Press. (atm)	0.7
Stage Pressure drop (atm)	0.003

Result Summary

Condenser / Top stage performance

Temperature:	21.4430707	K
Subcooled Temperature:		
Heat duty:	-0.5482588	kW
Subcooled duty:		
Distillate rate:	0.01947361	kmol/hr
Reflux rate:	1.59808753	kmol/hr
Reflux ratio:	82.0642517	
Free water distillate rate:		
Free water reflux ratio:		





6. ITER ISS 공정 시뮬레이션 Case 2

- The role of this Column 3 is to separate DT and T_2.
  - **Design specification 1 and Variable 1:**
    - ✓ 99% recovery of DT as a top distillate
    - ✓ Vary Distillate to feed ratio (0.001 to 1)
  - **Design specification 2 and Variable 2:**
    - ✓ 98.5% recovery of T_2 as a bottom product
    - ✓ Vary Reflux ratio (1 to 150)

	C3-F	T2	C3-DT
Temperature K	24.37407	24.95718	24.59887
Pressure atm	4	1.09	1.05
Mole Flow kmol/hr	0.090227	0.030148	0.060079
Mole Flow kmol/hr			
H2	9.56E-09	2.75E-29	9.56E-09
HD	0	0	0
HT	0	0	0
D2	0.000288	7.58E-16	0.000288
DT	**0.05994**	**0.0006**	0.059341
T2	**0.03**	0.029549	**0.00045**

DT recovery: 99% at top

T2 recovery: 98.5% at bottom

6. ITER ISS 공정 시뮬레이션 Case 2

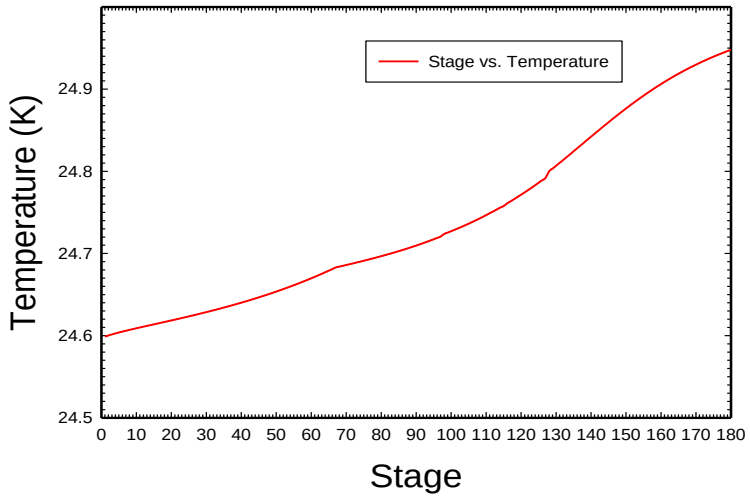
Column 3:

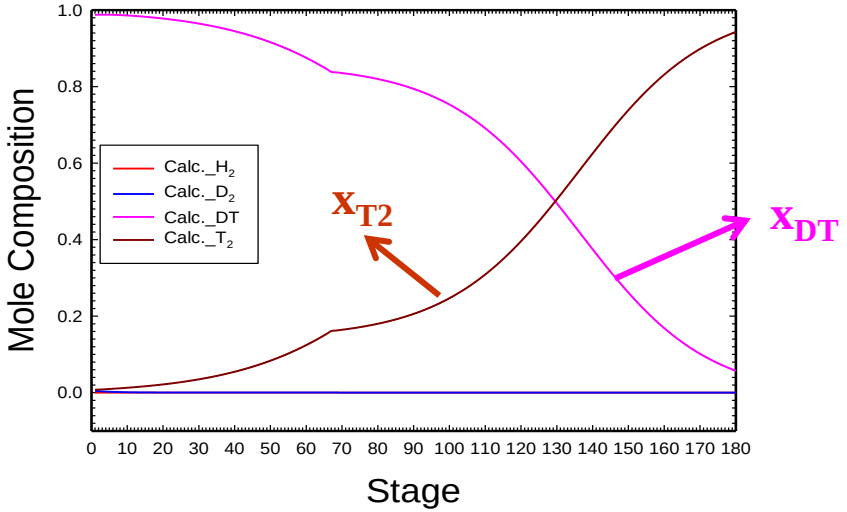
Column Name	Column 3
Reflux Ratio	**57**
Top Distillate Rate (mole/min)	0.6
Number of Stages	**180**
Feed Stage	67
Column Top Press. (atm)	1.05
Stage Pressure drop (atm)	0.04

Result Summary

Condenser / Top stage performance

Temperature:	24.5988549	K
Subcooled Temperature:		
Heat duty:	-1.2950885	kW
Subcooled duty:		
Distillate rate:	0.05887979	kmol/hr
Reflux rate:	3.32975485	kmol/hr
Reflux ratio:	56.5517387	
Free water distillate rate:		
Free water reflux ratio:		





6. ITER ISS 공정 시뮬레이션 Case 2

- In stream T2, expected T2 mole % is not less than 90%.
- We have obtained T2 mole % more than 94 mole%.

Stream Name	T_2	
Component	Mole %	
	Ref.	**Result**
H_2	Trace	0.00
HD	Trace	0.00
HT	Trace	0.00
D_2	Trace	0.00
DT	10.00	5.74
T_2	**90.00**	**94.26**
Total	100.00	100.00
Temperature (K)	26.40	24.95
Pressure (ATM)	1.08	1.09
Flow (kmol/hr)	0.030	0.031

6. ITER ISS 공정 시뮬레이션 Case 2

- The role of this Column 4 is to separate D_2 and DT.
  - **Design specification 1 and Variable 1:**
    - ✓ 99% recovery of D_2 as a top distillate
    - ✓ Vary Distillate to feed ratio (0.001 to 1)
  - **Design specification 2 and Variable 2:**
    - ✓ 99.9% recovery of T_2 as a bottom product
    - ✓ Vary Reflux ratio (1 to 150)

	C4-F	D2	C4-DT
Temperature K	20	23.0995246	23.1596917
Pressure atm	1.1	0.8	0.803
Mole Flow kmol/hr	0.07029931	0.06954111	0.0007582
Mole Flow kmol/hr			
H2	2.13E-06	2.13E-06	5.39E-12
HD	4.03E-08	4.03E-08	5.48E-19
HT	0.00059999	0.00059995	4.47E-08
D2	**0.0696353**	**0.0689389**	0.00069635
DT	**6.1855E-05**	6.1854E-08	**6.1793E-05**
T2	1.4384E-08	1.0171E-12	1.4383E-08

D2 recovery: 99% at top

DT recovery: 99.9% at bottom

6. ITER ISS 공정 시뮬레이션 Case 2

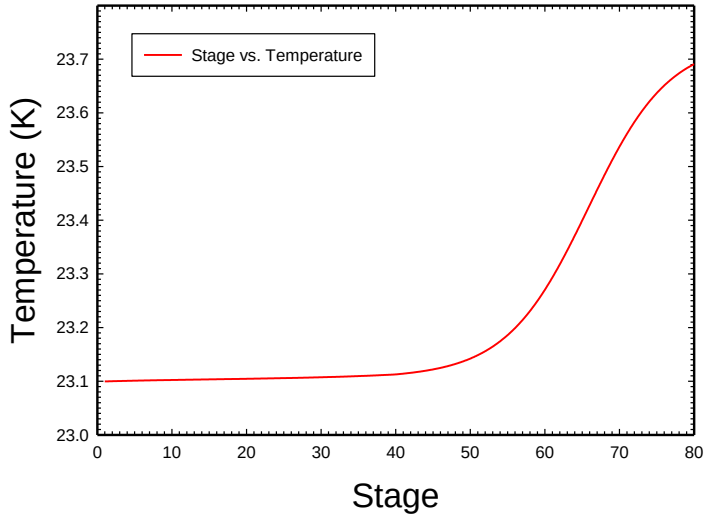
Column 4:

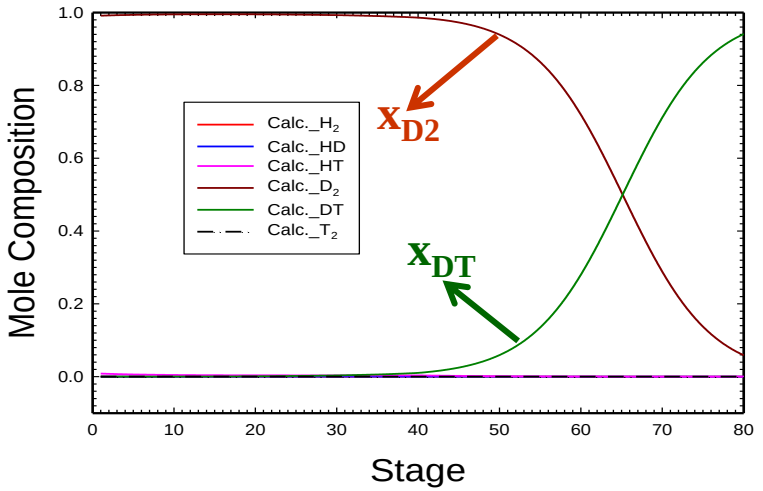
Column Name	Column 4
Reflux Ratio	13
Top Distillate Rate (mole/min)	1.17
Number of Stages	80
Feed Stage	40
Column Top Press. (atm)	0.8
Stage Pressure drop (atm)	0.003

Result Summary

Condenser / Top stage performance

Temperature:	23.0995961	K
Subcooled Temperature:		
Heat duty:	-0.3691852	kW
Subcooled duty:		
Distillate rate:	0.07024015	kmol/hr
Reflux rate:	0.93104476	kmol/hr
Reflux ratio:	13.2551641	
Free water distillate rate:		
Free water reflux ratio:		





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- Still we are trying to search for a new revised column configurations in order to reduce the content of T2 in DT product stream.

Stream Name	D_2		DT	
Component	Mole %		Mole %	
	Ref.	**Result**	**Ref.**	**Result**
H_2	Trace	0.00	Trace	0.00
HD	0.20	0.00	Trace	0.00
HT	1.60	0.85	Trace	0.00
D_2	**97.30**	**99.13**	1.30	0.49
DT	0.50	0.01	**98.70**	**98.74**
T_2	200 ppm	0.00	4ppm	0.76
Total	100.00	100.00	100.00	100.00
Temperature (K)	22.90	23.10	24.50	23.73
Pressure (ATM)	0.80	0.80	1.04	0.80
Flow (kmol/hr)	0.105	0.070	0.063	0.059

Should reduce the T2 content !!

감사합니다