추출탑을 이용한 에너지 절감: 23BDO+Water System

2017년 12월 25일(월)

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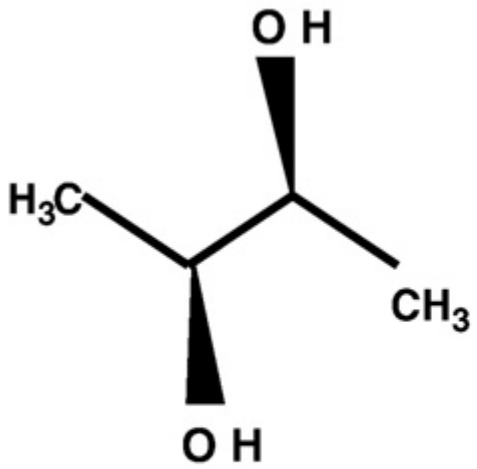
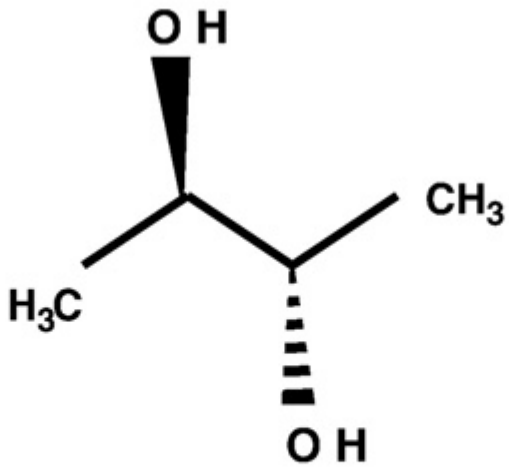
조 정 호

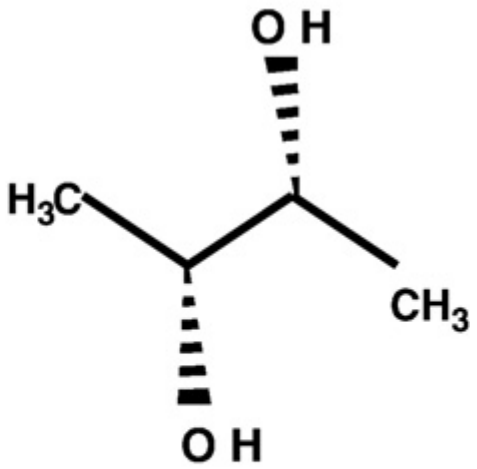
Stereo Isomers of 2,3-butanediol:



L-(+)-2,3-BD
Dextrorotatory form
(2S,3S)



meso-2,3-BD
Optically inactive form



D-(-)-2,3-BD
Levorotatory form
(2R,3R)

Other names:

- **2,3-Butylene glycol**
- **2,3-Dihydroxybutane**
- **Dimethylethylene glycol**
- **MW=90.12**

Applications of 2,3-butanediol

- Synthetic rubber
- Anti-freeze agents
- Solvents
- Plastics
- Flavoring agent in food products when it is converted to diacetyl
- Liquid fuel additive when it is converted to methyl ethyl ketone (heating value: 27,198 J/g; for example, HV of ethanol = 29,055 J/g)

Mixed Products in Fermentation Broth

- Acetic acid
- Acetoin
- 2,3-butanediol
- Ethanol
- Lactic acid

Feedstock Information

	Feed
Stream no.	**103**
Stream	T-101 FEED
Temperature	33.83
Pressure	0.50
Total Mass Rate	41538.96
Liquid Weight Fraction	0.00
(wt%) Weight. percent	
N2	0.00
H2	0.00
H2O	**93.86**
1BUTENE	0.00
13BD	0.00
C2BUTENE	0.00
IBUTALD	0.00
ETHANOL	0.09
MEK	0.00
FORMIC	0.00
ACETIC	0.03
ACETOIN	0.24
23BDO	**5.78**
LACTIC	0.01
SUCCINIC	0.00
NC20	0.00

Product Specifications:

- 23BDO Product Purity: Not Less Than 90 wt%
- 23BDO Recovery Ratio: Not Less Than 99%

Recovery of 2,3-butanediol:

- Pervaporation
- Membrane Distillation
- Vacuum Membrane Distillation
- Solvent Extraction

Recovery of 2,3-butanediol:

Methods	Descriptions
Pervaporation	Selective diffusion of a component through a non-porous membrane due to a concentration gradient
Membrane distillation	A process of evaporation through a porous hydrophobic membrane. Membrane: Liquid-vapor interface The transport of vapor is accomplished by a temperature gradient between the membrane and the condensing surface.
Vacuum membrane distillation	PTFE (microporous) membrane allowed water vapor to pass, while retaining 2,3-BDO
Solvent extraction	By using alcohols or esters as solvents Other solvents: ethyl acetate, diethyl ether, and n-butanol Salting-out effect (potassium chloride)

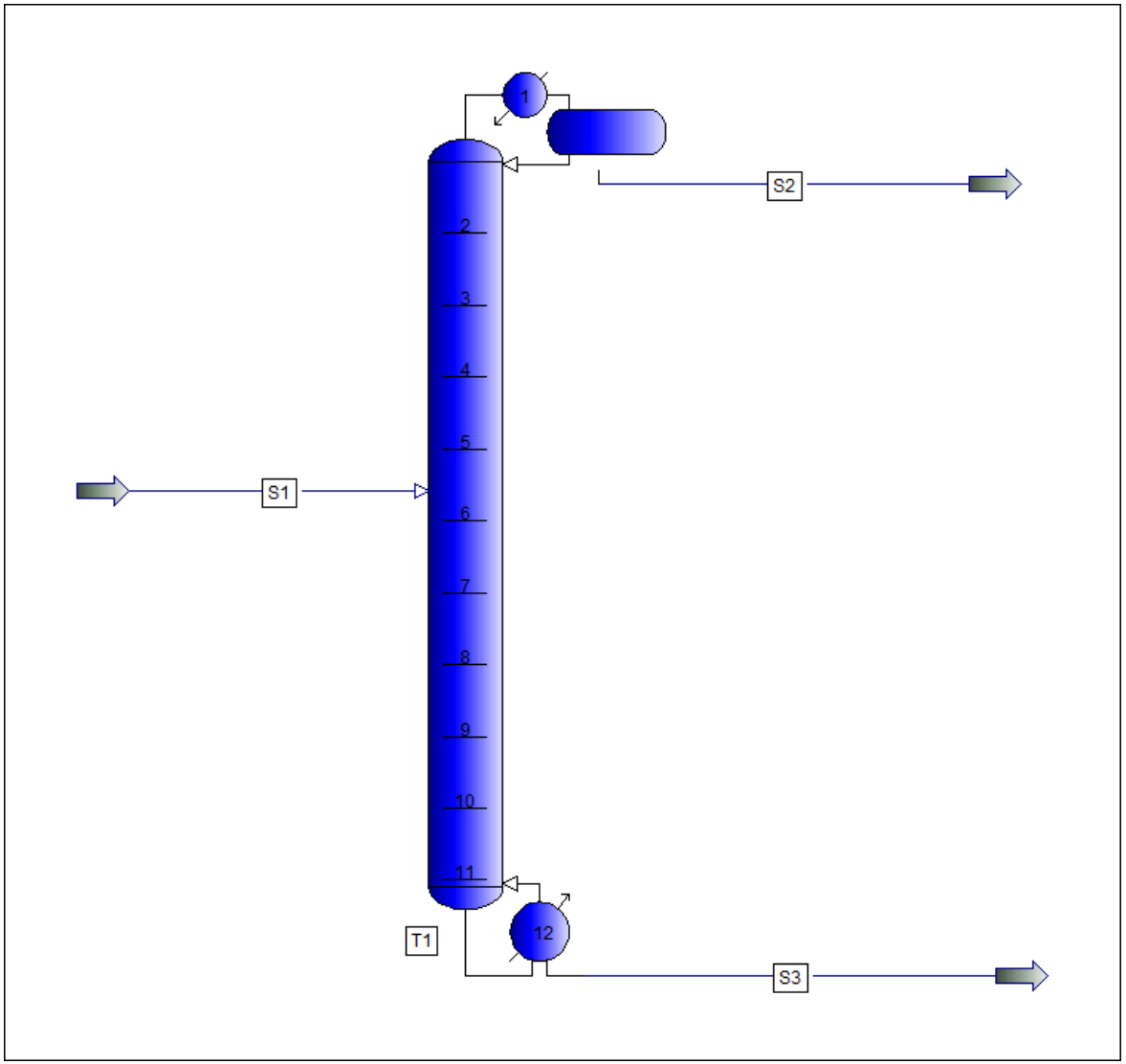
Comparison between Separation Methods:

Methods	Advantages	Disadvantages
Pervaporation	• Low energy consumption • Low operating temperature (can be coupled with biological process)	• Membranes are relatively expensive • Low product concentration • Fouling
Membrane distillation	• The cost of running the unit is low. • Operate at ambient pressures. • Can operate at lower temperatures.	• Fluxes are lower than in other separation processes for industrial applications. • Fouling • Low product concentration
Solvent extraction	• Low operating temperature • Easy to perform	• Require large amounts of solvent

Conventional Distillation Method is Not Good….

- Conventional distillation is not a good suggestion for 2,3-butanediol recovery because:
  - High boiling point (180~184^{o}C)
  - High affinity for water
  - Diluted in water and higher utility cost for separation

Conventional Distillation Simulation Using PRO/II:



Conventional Distillation Simulation Using PRO/II:

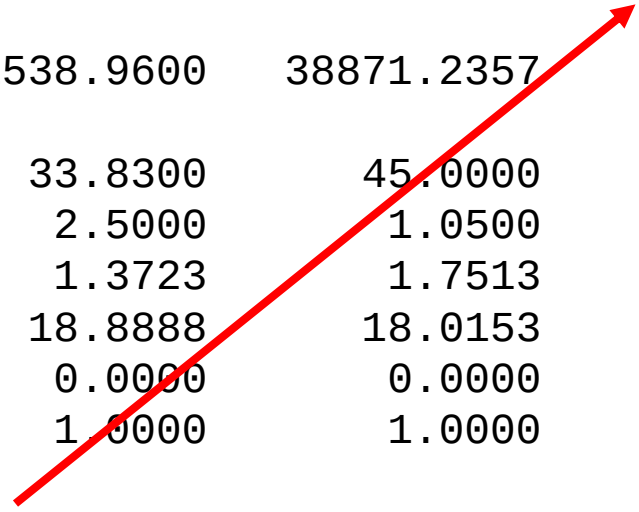
COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE BAR	NET FLOW RATES LIQUID KG-MOL/HR	NET FLOW RATES VAPOR KG-MOL/HR	NET FLOW RATES FEED KG-MOL/HR	NET FLOW RATES PRODUCT KG-MOL/HR	HEATER DUTIES M*KCAL/HR
1C	**45.0**	**1.05**	6473.0			2157.7L	**-92.9528**
2	**104.8**	**1.20**	7191.2	8630.7			
3	105.3	1.22	7194.6	9348.9			
4	105.8	1.24	7198.0	9352.3			
5	106.2	1.26	7200.7	9355.6			
6	106.8	1.28	9711.0	9358.4	2199.1L		
7	107.2	1.30	9716.3	9669.5			
8	107.7	1.32	9721.6	9674.9			
9	108.1	1.34	9725.6	9680.2			
10	108.7	1.36	9644.7	9684.2			
11	**119.0**	**1.38**	8665.1	9603.2			
12R	**156.1**	**1.40**		8623.6		41.4L	**93.6055**

Too much reboiling heat is required.

Stream Summary:

STREAM ID	S1	S2	S3
NAME			
PHASE	LIQUID	LIQUID	LIQUID
THERMO ID	WILS01	WILS01	WILS01
FLUID RATES, KG/HR			
1 H2O	39138.0081	38871.2357	266.7724
2 23BTD	**2400.9519**	4.8194E-06	**2400.9519**
TOTAL RATE, KG/HR	41538.9600	38871.2357	2667.7243
TEMPERATURE, C	33.8300	45.0000	156.0535
PRESSURE, BAR	2.5000	1.0500	1.4000
ENTHALPY, M*KCAL/HR	1.3723	1.7513	0.2737
MOLECULAR WEIGHT	18.8888	18.0153	64.3613
WEIGHT FRAC VAPOR	0.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	1.0000	1.0000	1.0000



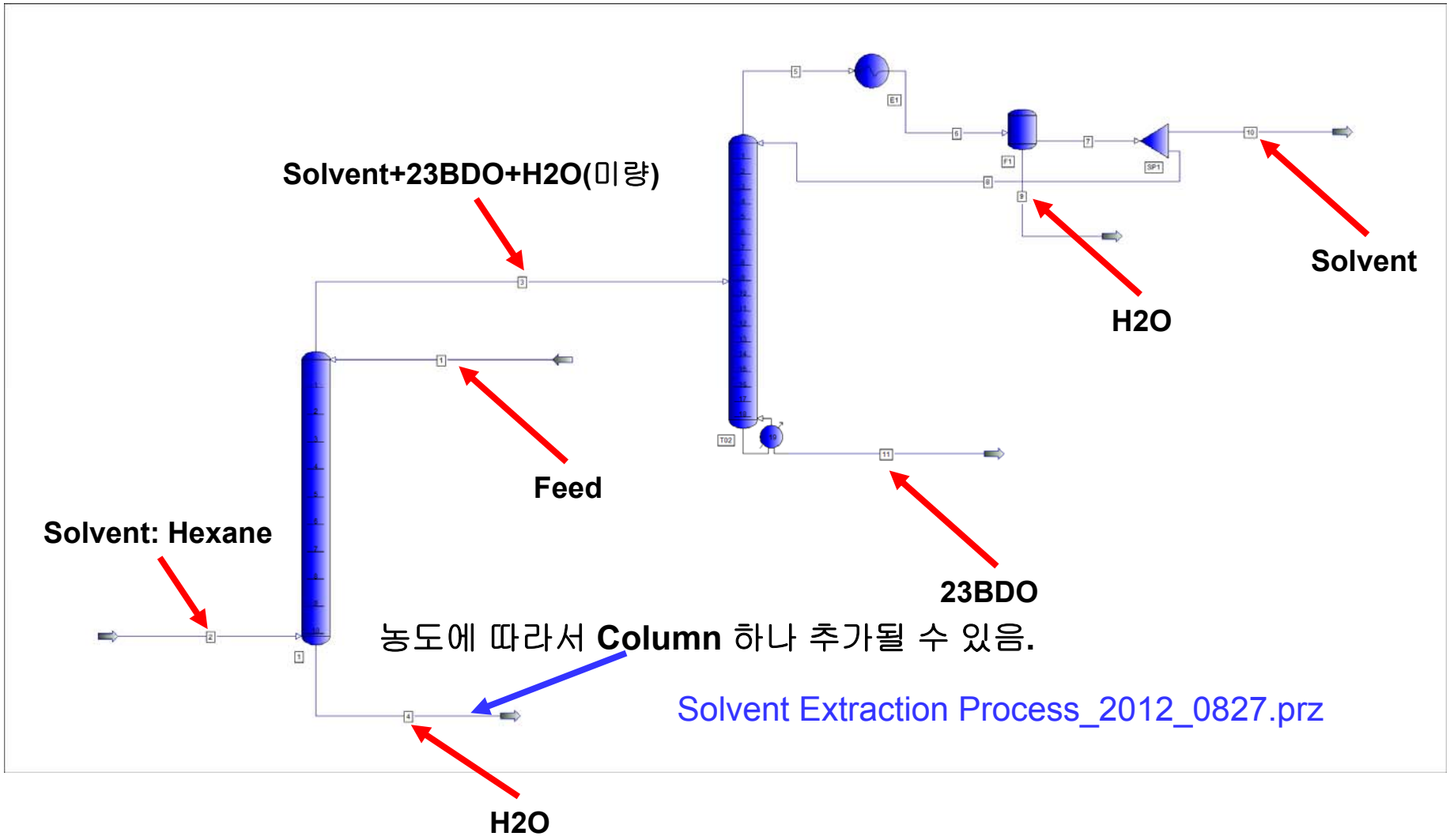
23BDO Recovery at Column BTMS: ~100%

Stream Summary:

STREAM ID		S1	S2	S3
	NAME			
	PHASE	LIQUID	LIQUID	LIQUID
THERMO ID		WILS01	WILS01	WILS01
FLUID WEIGHT PERCENTS				
1	H2O	94.2200	100.0000	10.0000
2	**23BTD**	5.7800	1.2398E-08	**90.0000**
TOTAL RATE, KG/HR		41538.9600	38871.2357	2667.7243
TEMPERATURE, C		33.8300	45.0000	156.0535
PRESSURE, BAR		2.5000	1.0500	1.4000
ENTHALPY, M*KCAL/HR		1.3723	1.7513	0.2737
MOLECULAR WEIGHT		18.8888	18.0153	64.3613
WEIGHT FRAC VAPOR		0.0000	0.0000	0.0000
WEIGHT FRAC LIQUID		1.0000	1.0000	1.0000

23BDO Purity at Column BTMS: 90wt%

Solvent Extraction:



Extractor Profile:

COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE BAR	NET FLOW RATES KG/HR L2	NET FLOW RATES KG/HR L1	NET FLOW RATES KG/HR FEED	NET FLOW RATES KG/HR PRODUCT	HEATER DUTIES M*KCAL/HR
1	33.8	9.80	40092.1		41539.0L	23195.7L	
2	33.8	9.89	39535.0	21748.9			
3	33.8	9.98	39300.6	21191.9			
4	33.8	10.07	39198.4	20957.5			
5	33.8	10.16	39153.2	20855.2			
6	33.8	10.24	39133.0	20809.9			
7	33.8	10.33	39124.0	20789.7			
8	33.6	10.42	39119.8	20780.6			
9	33.1	10.51	39117.5	20776.4			
10	31.3	10.60		20774.2	20769.5L	39112.8H	

Column Profile:

COLUMN SUMMARY

TRAY	TEMP DEG C	PRESSURE BAR	NET FLOW RATES KG-MOL/HR LIQUID	VAPOR	FEED	PRODUCT	HEATER DUTIES M*KCAL/HR
1	75.6	1.20	66.0		58.2L	300.6V	
2	78.1	1.21	61.1	308.4			
3	81.0	1.22	57.1	303.4			
4	83.3	1.23	54.7	299.5			
5	84.8	1.24	53.4	297.1			
6	85.7	1.26	52.7	295.8			
7	86.2	1.27	52.2	295.1			
8	86.5	1.28	51.7	294.6			
9	87.0	1.29	48.7	294.1			
10	89.2	1.30	371.0	291.1	269.1L		
11	106.0	1.31	356.3	344.3			
12	115.8	1.32	347.7	329.6			
13	118.9	1.33	336.5	321.0			
14	125.7	1.34	299.4	309.8			
15	152.6	1.36	253.3	272.7			
16	177.7	1.37	246.3	226.5			
17	186.6	1.38	246.6	219.6			
18	189.3	1.39	246.9	219.9			
19R	190.2	1.40		220.2		26.7L	2.8692

Condenser Summary:

UNIT 3, 'E1'

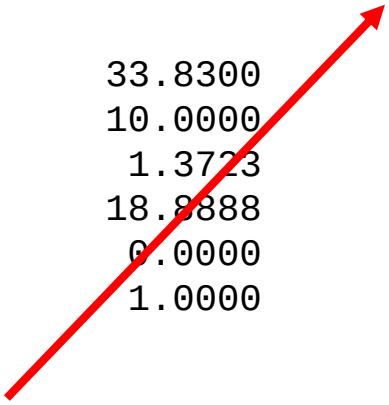
OPERATING CONDITIONS

DUTY, M*KCAL/HR	2.527

HOT SIDE CONDITIONS	INLET	OUTLET
FEED	5	
LIQUID PRODUCT		6
VAPOR, KG-MOL/HR	300.565	
K*KG/HR	25.803	
CP, KCAL/KG-C	0.406	
LIQUID, KG-MOL/HR		300.565
K*KG/HR		25.803
CP, KCAL/KG-C		0.557
TOTAL, KG-MOL/HR	300.565	300.565
K*KG/HR	25.803	25.803
CONDENSATION, KG-MOL/HR		300.565
TEMPERATURE, C	75.623	45.000
PRESSURE, BAR	1.200	1.200

Stream Summary:

STREAM ID	1	**2**	3	4
NAME				
PHASE	LIQUID	LIQUID	LIQUID	LIQUID
THERMO ID	NRTL01	NRTL01	NRTL01	NRTL01
FLUID RATES, KG/HR				
1 H2O	39138.0081	0.0000	26.2177	39111.7666
2 23BTD	2400.9519	0.0000	2400.6384	0.4841
3 NC6	0.0000	**20769.4800**	20768.8910	0.5361
TOTAL RATE, KG/HR	41538.9600	**20769.4800**	23195.7471	39112.7867
TEMPERATURE, C	33.8300	25.0000	33.8300	31.2547
PRESSURE, BAR	10.0000	11.0000	9.8000	10.6000
ENTHALPY, M*KCAL/HR	1.3723	0.2764	0.4229	1.2258
MOLECULAR WEIGHT	18.8888	86.1771	86.1990	18.0157
WEIGHT FRAC VAPOR	0.0000	0.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	1.0000	1.0000	1.0000	1.0000



Solvent

Stream Summary:

STREAM ID	5	6	7	8
NAME				
PHASE	VAPOR	LIQUID	LIQUID	LIQUID
THERMO ID	WILS01	SRKK01	SRKK01	NRTL01
FLUID RATES, KG/HR				
1 H2O	26.2418	26.2418	6.3058	1.2262
2 23BTD	3.9589E-10	3.9589E-10	1.0672E-10	2.0753E-11
3 NC6	25776.3409	25776.3409	25776.3405	5012.4200
TOTAL RATE, KG/HR	25802.5827	25802.5827	25782.6463	5013.6463
TEMPERATURE, C	75.6231	45.0000	45.0000	45.0000
PRESSURE, BAR	1.2000	1.2000	1.2000	1.2000
ENTHALPY, M*KCAL/HR	3.1263	0.5997	0.5987	0.1164
MOLECULAR WEIGHT	85.8468	85.8468	86.0975	86.0975
WEIGHT FRAC VAPOR	1.0000	0.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	0.0000	1.0000	1.0000	1.0000

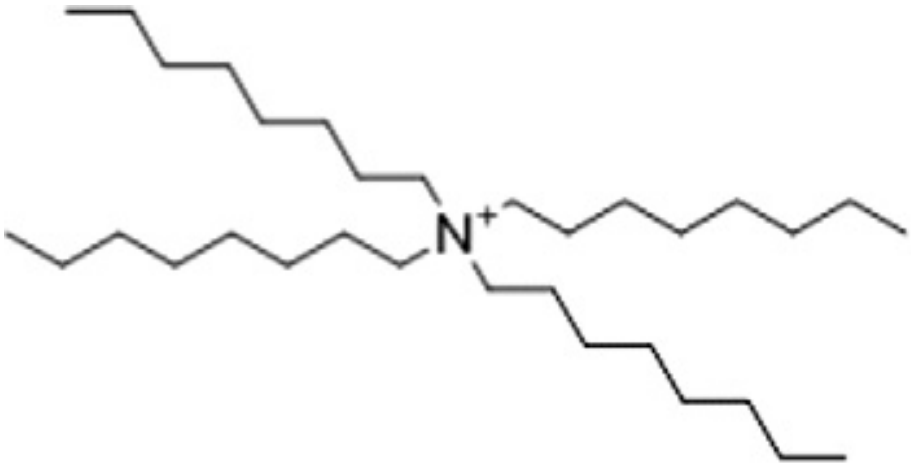
Stream Summary:

STREAM ID	9	10	11
NAME			
PHASE	LIQUID	LIQUID	LIQUID
THERMO ID	SRKK01	NRTL01	WILS01
FLUID RATES, KG/HR			
1 H2O	19.9360	5.0796	1.2009
2 23BTD	2.8917E-10	8.5968E-11	2400.6384
3 NC6	4.1809E-04	20763.9204	0.0154
TOTAL RATE, KG/HR	19.9364	20769.0000	2401.8548
TEMPERATURE, C	45.0000	45.0000	190.1845
PRESSURE, BAR	1.2000	1.2000	1.4000
ENTHALPY, M*KCAL/HR	9.9890E-04	0.4823	0.2880
MOLECULAR WEIGHT	18.0156	86.0975	89.9422
WEIGHT FRAC VAPOR	0.0000	0.0000	0.0000
WEIGHT FRAC LIQUID	1.0000	1.0000	1.0000

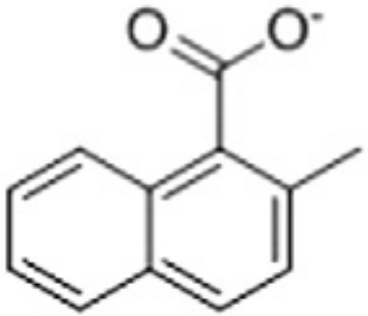
13BDO recovery>99.9%

Suitable Solvent List for the Recovery of 23BOD(1):

- Tetraoctyl ammonium 2-methyl-1-naphthoate
  - (Liquid+liquid) equilibrium data for the separation of 2,3-butanediol from aqueous streams using tetraoctyl ammonium and 2-methyl-1-naphthoate
  - J. Chem. Thermodynamics

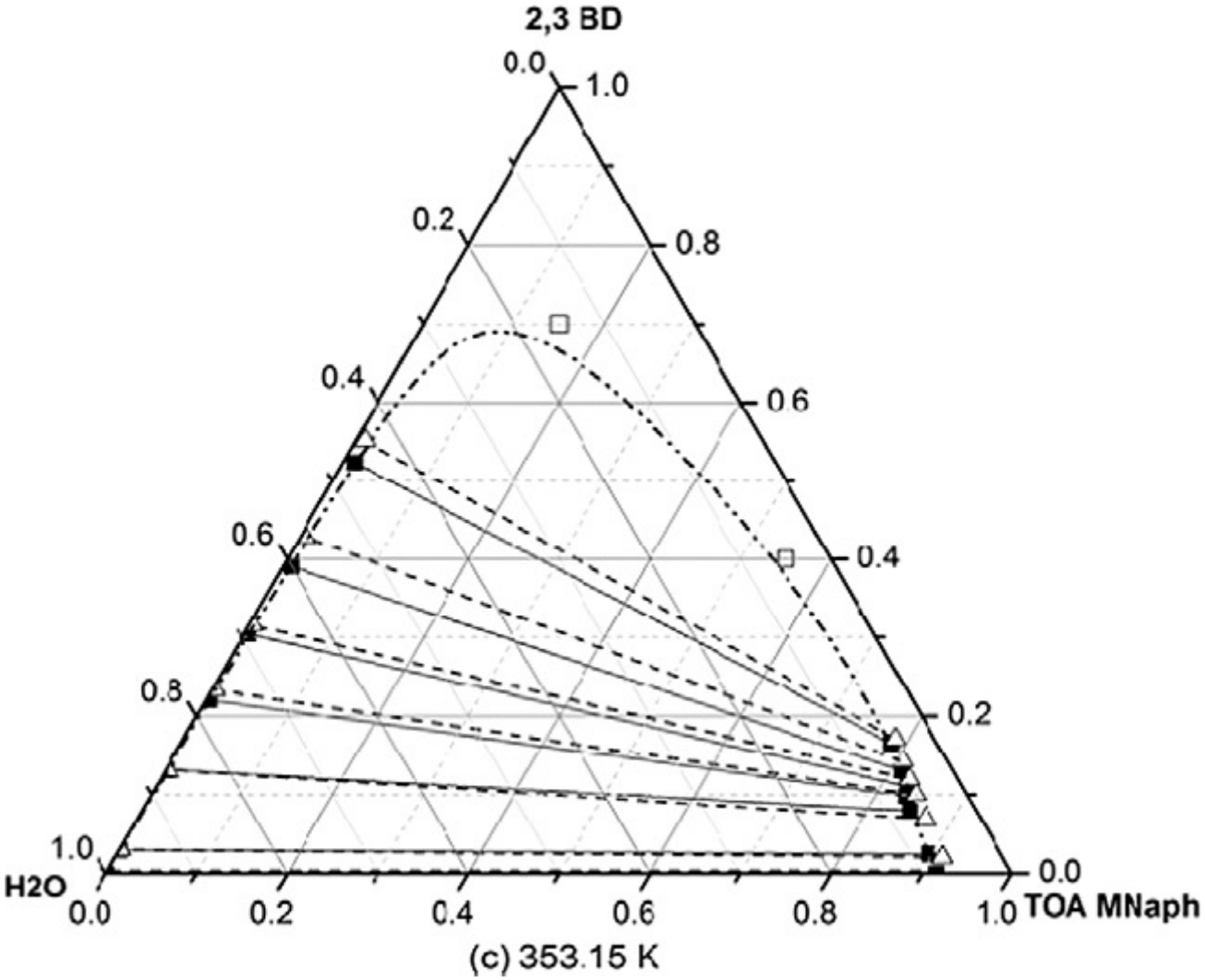


tetraoctyl ammonium



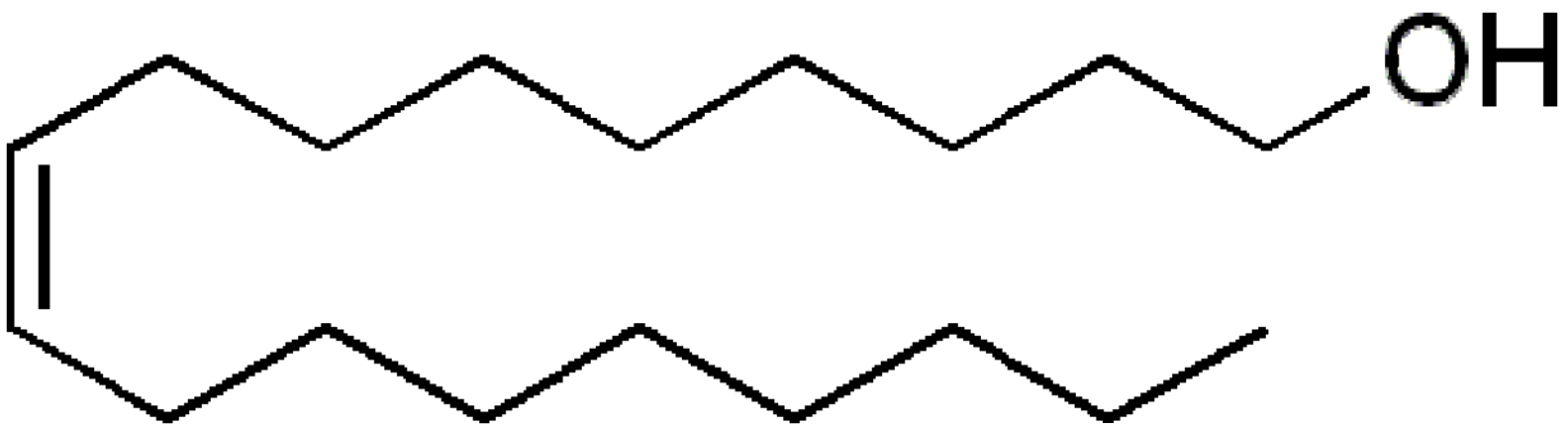
2-Methyl-1-naphthoate

Ternary LLE for 23BDO/H_2O/Solvent

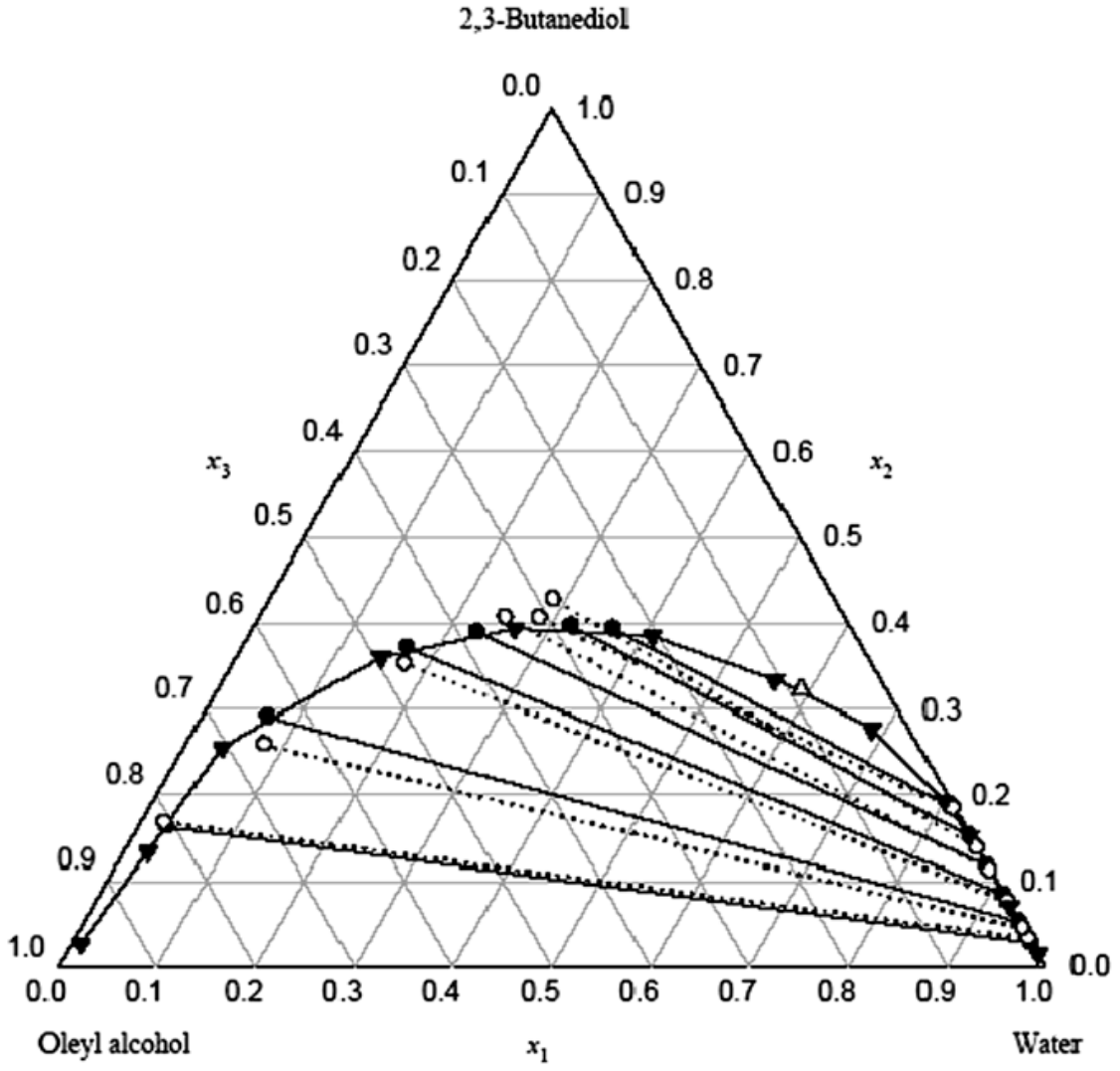


Suitable Solvent List for the Recovery of 23BOD(2):

- Oleyl alcohol
  - (Liquid+liquid) equilibria for (water + 2,3-butanediol + oleyl alcohol) at T = (300.2, 307.2 and 314.2) K
  - J. Chem. Thermodynamics



Ternary LLE for 23BDO/H_2O/Solvent



새로운 Solvent를 이용한 추출공정 전산모사:

➢ 현재 문제점

- PRO/II 순수성분 DB에 내장되어 있지 않다.
- TDM을 활용하여 구조식으로부터 순수성분의 물성 추산
- 삼성분계(23BDO/H2O/Solvent간) LLE 실험 데이터 Regression 수행하여 NRTL 또는 UNIQUAC Parameter Regression 해야 함
- 상기 과정이 완결되면 Solvent 성능 평가 및 후속 증류공정에 대한 전산모사 가능함
- 추출탑 사이징: GTC의 정경호 부장
- 후속 증류공정 사이징 작업을 통한 총 투자비 및 운전비용 산출 가능함

THANK YOU