Techno-economic analysis of the production of epichlorohydrin from glycerol.

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Cost analysis

Equipment

1. **Washing unit**

The Washing operation was considered to be like a screw, so the cost can be estimated as:

$$C_{Wash} = 28,899 \cdot \left(\frac{Load_{(Solids+water)}(lb/h)}{277 \cdot d_{screw}(in) - 494} \right)$$

The typical d_{screw} is taken to be 24.[1] The water used inside this unit is half the load of solids.

If necessary, the given cost has to be updated to the current year by the next expression:

$$C_{\$-2014} = C_{\$-año} \cdot \frac{\text{IM\&}S_{2014}}{\text{IM\&}S_{\text{año}}} \cdot \frac{IL_{España}}{IL_{País}}$$

Where:

- $C_{€-2014}$: coste estimado en euros para el año actual.
- C_{Xyear}: coste estimado en la divisa X para el año dado.
- $\text{IM\&}S_{2014}$: Marshall and Swift (1.708,49).
- $\text{IM\&}S_{\text{year}}$: Marshall and Swift
- $IL_{España}$: Spanis index (1,2).
- $IL_{País}$: County index. USA (1,0)

2. **Grinding unit**

The grinding cost was estimated using a Rod mill to be $2,080,000 using a diameter of 12.5 ft.[2] The best efficiency is achieved for d = 12.5 ft [3]

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3. **Vessels**

In order to calculate the sizes of the equipment in the plant, the residence times in the vessels are used. The sizes of the premix tank, the gelatinization column, the liquefaction tank, the saccarification tank, the floculation unit and the storage tanks before and after the fermentors are calculated with the following formula:

$$Volume = \left(\frac{\dot{m}}{\rho}\right)\tau$$

ρ is taken to be 1000 Kg/ m3. τ is the residence time (in sec).

The diameter of the vessels is calculated considering spherical heads for the vessels as well as a length L = $4D_c$ so

$$D_C = \sqrt[3]{\frac{6 \cdot Volume}{7 \cdot \pi}}$$

and the weight is calculated as

$$W = \rho_{steel}\left(\pi\left[\left(\frac{D_c}{2}+e\right)^2 - \left(\frac{D_c}{2}\right)^2\right]L + \frac{4}{3}\pi\left[\left(\frac{D_c}{2}+e\right)^3 - \left(\frac{D_c}{2}\right)^3\right]\right)$$

where the thickness *e* (m) is taken to be [4]

e = 0.0023 + $0.003D_c$

Column Col1 is a vertical vessel and its cost will be estimated as:

$$C_{column} = 62.379 \,.\, W^{0.878}$$

Weight is in Kg.

Cost correlation from[2]:

Columns made of stainless steel; medium size; no internals)

The above correlation will hold for all vertical vessels.

The cost of the **storage tanks** will be calculated as a vertical **tank**[2] (cone roof, and flat bottom made of stainless steel)

$$C_{tank} = 6{,}839.8 \,.\, V(m^3)^{0.65}$$

Volume is in m^3

4. **Fermentation tanks**

The cost correlation is taken to be:

$$C_{Fermentors} = 78809\,.Volume^{0.53}$$

$$Volume = \left(\frac{\dot{m}}{\rho}\right)\tau$$

Volume is in m^3.

Cost correlation updated from[2]:

A Fermenter Reactor made of Stainless steel 316 operating up to 25 psi)

5. **Mechanical Separation**

The mechanical separation is considered as a centrifuge (Centrifugal Separator Bottom Driven ss316[2]):

$$C_{MechSep} = 892 \cdot d \cdot \left(\frac{Load(gal/\min)}{200(gal/\min)}\right)$$

d is typically 24 in and the maximum capacity of 200 gal/min for a single centrifuge is taken from Walas (1990).

$$C_{MechSep}(24\ inch) = 25{,}700\ \$_{2014}$$

6.-Compressor costs

Centrifugal compressors have been considered and tow correlations will be used depending on the final pressure of the stream:[2]

For Low pressures till 125 psi $C_{compressor} = 335.27\,.P\ (kW) + 36{,}211$

For pressure till 1000psi $C_{compressor} = 2534.80\,.P\ (kW)^{0.8}$

7.-Gasifiers

They are priced as if they were boilers pul. Coal Fired[2]

Low pressure (150 psi sat) $C_{Gasif} = 1{,}164{,}817\,.\ Flow\ (kg/s)^{0.698}$

Medium pressure (600 psi 750 F) $C_{Gasif} = 1{,}592{,}418\,.\ Flow\ (kg/s)^{0.681}$

High pressure (1500 psi 950 F) $C_{Gasif} = 2{,}179{,}923\,.\ Flow\ (kg/s)^{0.684}$

8.-**Cyclons**

They are priced by the gas flow rate [2]

$$C_{cyclon} = 4{,}463\ .Flow\ (m^3/s)^{0.8945}$$

9.- **Electrostatic precipitator and filter**

They are priced by the gas flow rate [2]

$$C_{EP} = 5{,}111.6\ .Flow\ (m^3/s) + 149{,}832$$

$$C_{Filter} = 5{,}497.4\ .Flow\ (m^3/s) + 18{,}219$$

10.- Wet Scrubber

They are priced by the gas flow rate [2]

$$C_{Scrubber} = 4796.1 \cdot Flow(m^3/s) + 10173$$

11. Molecular sieves and PSA systems.

The **molecular sieves** are cost estimated using the price of the adsorbent and vertical vessels. Two beds are needed to ensure continuous operation. We use an over-design factor of 10% for safety reasons.Molecular sieves with a bulk density of 45 lb/ft^3. [5]

(source:

$$\text{Volume of bed} = \frac{\text{Bed size}}{\text{Bulk density}} = \frac{1.1 \cdot \text{Mass(Kg)}}{41.5 \frac{\text{lb}}{\text{ft}^3} \cdot 0.454\ \frac{\text{Kg}}{\text{lb}} \cdot (\frac{1\ \text{ft}}{0.3048\ \text{m}})^3}$$

Molecular sieves data:

The price is around 1550 $\$_{2015}$ per ton for zeolite 13x[6], 1700 $\$_{2015}$/t for 5A [7] or 1175 $\$_{2015}$/t for silica gel[8] The molecular sieves are assumed to be a combination of two vertical vessels and the cost will be estimated as[2]:

$$C_{MS} = 2.(\cos t\ of\ bed + 56.181\ W^{0.878})$$

Weight is in Kg.

12. Heat exchangers

WE use various correlations as a function of their size and type. The basic features are Heat Exchanger, Stainless steel 316 working up to 150 psig. The type of the heat exchanger is either reboiler or Shell / Tube Fixed U, small, medium and big): [2]

$$C_{reboiler} = 815.55\ .\ A(m^2) - 6601.9$$

$C_{Heat\ Ex} = 293.59\ .A\ (m^2)^{1.4915}$ $A < 25m^2$

$C_{Heat\ Ex} = 1{,}593.8\ .\ A(m^2) + 2{,}584.2$ $25 < A < 140m^2$

$C_{Heat\ Ex} = 22{,}234\ .A\ (m^2)^{0.4671}$ $A > 140m^2$

C in \$, A is the area in m^2.

13. Columns

The **distillation columns** are cost estimated as vertical vessels including the cost of the sieve plates.

The diameter of the columns is calculated as:[4]

$$D_C = 2\cdot\sqrt{\frac{1}{\pi}\cdot\frac{\text{Vapor rate(kg/s)}}{\rho_v\cdot(\text{vapor velocity(m/s)})}}$$

$$\text{Vapor rate(kg/s)} = (1+R)\cdot D$$

R is the reflux ratio and D is distillate withdrawn from top.

In case the diameter of the column is bigger than 3m the feed should be split into as many columns as those which allow a D_c of around 3m.[4]

$$vapor\ velocity(m.s) = 0.8\cdot \max vapor\ velocity = 0.8\cdot 0.3048\cdot 0.3\cdot\sqrt{\frac{\rho_L-\rho_v}{\rho_v}}$$

(0.8 is the fraction of the flooding velocity:[4]

($0.3\cdot\sqrt{\frac{\rho_L-\rho_v}{\rho_v}}$ ft /s is the maximum vapor velocity[9] corresponding to a plate separation of 2 ft

(0.3048 if because 0.3 is given for a velocity in ft/s instead of m/s.

The number of plates for each column is calculated as:

$$n_{Plates} = \text{Round}\left(\frac{\dfrac{\ln\left(\dfrac{\xi_{etho}(1-\xi_{wa})}{\xi_{wa}(1-\xi_{etho})}\right)}{\ln(\alpha_{etho/wa})}-1}{Efficiency}+1\right)$$

Efficiency = $0.5/(0.3\cdot\alpha_{etho/wa})^{0.25}$ [10]

The height of the column will be

$$H = n_{Plates}\cdot Esp + 4\cdot 1.5$$

Esp is the separation between plates and is commonly taken as 0.6m. [10] The factor 4 times 1.5m is a consideration for space above the top plate and below the bottommost plate.

Since the column thickness is small compared to its diameter, we can calculate its weight using:

$$W = \rho_{steel} \cdot \left(\pi \cdot D_C \cdot e \cdot H + \frac{4}{3} \cdot \pi \cdot \left[\left(\frac{D_C}{2} + e \right)^3 - \left(\frac{D_C}{2} \right)^3 \right] \right)$$

$\rho_L = 950 kg / m^3$ (Liquid phase density)

$\rho_v = \frac{P \cdot M_{Water-EtOH}}{R \cdot T} (kg / m^3)$ (Gas phase density)

The bottoms pressure and temperature is used for calculating the vapor density.

Thickness calculation:[2]

$$P > atm \quad t = 0.0032 + \frac{P.D_c}{2.S.E - 0.2P}$$

$$P < atm \quad t = 0.0032 + 4.\frac{D_c}{2}.\sqrt{\frac{P_{out}}{S}}$$

Corrosion allowance, 0.0032m (from 2 to 4 mm, typically 1/8 in = 3.2 mm is used)[2]

t (m): thickness

E: joint efficiency, equal to 1

P (psi): Design pressure – We have selected 1.5 times the working pressure since bottoms pressures is higher than atmospheric pressure

P_{out} (psi): Pressure outside the column (= atmospheric pressure). units consistent with those of S

S (psi): Design stress (S = 13300 psi for stainless steel working at 100ºC).[11]

D_c (m): column diameter

Another correlation for thickness:

t (m) = 0.0023 + 0.003D_c

where D_c is in m

The above correlation has been derived from a table of minimum thickness,[2]

The cost of the plates is given by [2]

$$Cost \;\; Plates(\$) = n_{Plates} \cdot 315 \cdot e^{0.72 \cdot D_C}$$

where D_c is in m

$C_{column} = 62.379 \, . W^{0.878} + Cost\ Plates$

Weight is in Kg.

References:

[1] Baasel, W.D. Preliminary Chemical Engineering Plant Design", Van Nostrand Reinhold, 2nd ed., New York, 1990

[2] Matche http://www.matche.com/equipcost/EquipmentIndex.html, (Accessed July 2014)

[3] www.mcintoshengineering.com (Accessed July 2014)

[4] Sinnott, R.K. Coulson and Richardson's Chemical Engineering, Vol 6, 3rd ed., Butterworth Heinemann, Singapore, 1999

[5] http://www.sigmaaldrich.com/Brands/Aldrich/Tech_Bulletins/AL_143/Molecular_Sieves.html) (Accessed 2009)

[6] (http://www.alibaba.com/product-detail/zeolite-catalyst-13x-for-hydrogen_1605925007.html?spm=a2700.7724857.35.1.CmlJlt (Accessed July 2015)

[7]http://www.alibaba.com/product-detail/Zeolita-5A-Beads_1357023920.html?spm=a2700.7724838.35.1.MrhIye (Accessed July 2015)

[8]http://www.alibaba.com/product-detail/silica-gel-packed beds_60045197042.html?spm=a2700.7724838.35.1.tdidtX. (Accessed July 2015)

[9] Branan, C.R. Rules of thumb for chemical engineers : a manual of quick, accurate solutions to everyday process engineering problems. 2nd ed,.Gulf Publishing Company, Texas 1998

[10] Douglas, J.M. Conceptual Design of Chemical Processes. McGraw Hill, International Editions, Singapore, 1988

[11] Walas, S.M. Chemical Process Equipment - *Selection and Design*. Butterworths Series in Chemical Engineering, Boston, 1990

Stream	1		2		3		4		5	
T (K)	293.15		375.60		292.80		378.57		423.97	
P (kPa)	100		10		10		10		100	
Total molar flow (kmol/h)	83.61		83.61		34.89		48.72		55.92	
Total mass flow (kg/h)	5,176.80		5,176.80		966.80		4,210.00		5,026.39	
Vapor fraction	0		0		0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.290	0.150	0.290	0.150	0.691	0.201	0.003	0.983	0.003	0.001
Water	0.172	0.050	0.172	0.050	0.309	0.799	0.074	0.016	0.064	0.013
Glycerol	0.538	0.800	0.538	0.800	0.000	0.000	0.923	0.001	0.804	0.824
Dichlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	8.70 E-5	1.25 E-4
Monochlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.064	0.078
Hexanoic Acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.065	0.084
Hydrogen Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Stream	6		7		8		9		10	
T (K)	383.15		293.00		453.32		419.34		383.15	
P (kPa)	100		100		350		760		350	
Total molar flow (kmol/h)	55.92		100.83		100.83		100.83		100.83	
Total mass flow (kg/h)	5,026.39		3,657.79		3,657.79		3,657.79		3,657.79	
Vapor fraction	0		1		1		1		1	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.003	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.064	0.013	0.010	0.995	0.010	0.995	0.010	0.995	0.010	0.995
Glycerol	0.804	0.824	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	8.70 E-5	1.25 E-4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Monochlorohydrins	0.064	0.078	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hexanoic Acid	0.065	0.084	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hydrogen Chloride	0.000	0.000	0.990	0.005	0.990	0.005	0.990	0.005	0.990	0.005

Stream	11		12		13	
T (K)	453.32		383.15		383.15	
P (kPa)	760		760		760	
Total molar flow (kmol/h)	100.83		12.12		144.63	
Total mass flow (kg/h)	3,657.79		357.23		8,326.95	
Vapor fraction	1		1		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.010	0.995	0.386	0.231	0.622	0.195
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.000	0.000	0.000	0.000	0.311	0.697
Monochlorohydrins	0.000	0.000	0.000	0.000	0.025	0.047
Hexanoic Acid	0.000	0.000	0.000	0.000	0.025	0.051
Hydrogen Chloride	0.990	0.005	0.614	0.769	0.017	0.010

Stream	14		15		16		17		18	
T (K)	337.15		333.99		482.14		482.15		333.99	
P (kPa)	100		100		100		100		100	
Total molar flow (kmol/h)	144.63		137.45		7.18		7.20		48.15	
Total mass flow (kg/h)	8,326.95		7512.72		814.22		816.39		5,710.80	
Vapor fraction	0		0		0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.622	0.195	0.655	0.216	8.49 E-18	1.35 E-18	0.000	0.000	0.093	0.014
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.311	0.697	0.327	0.772	6.85 E-4	7.79 E-4	6.48 E-4	7.38 E-4	0.907	0.986
Monochlorohydrins	0.025	0.047	1.84 E-14	3.72 E-14	0.494	0.481	0.503	0.491	0.000	0.000
Hexanoic Acid	0.025	0.051	1,34 E-7	2.84 E-7	0.506	0.518	0.496	0.509	0.000	0.000
Hydrogen Chloride	0.017	0.010	0.018	0.012	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Epichlorohydrin	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Stream	19		20		21		22		23	
T (K)	333.99		333.99		298.15		298.15		366.10	
P (kPa)	100		100		100		100		100	
Total molar flow (kmol/h)	89.30		89.30		358.43		47.22		405.65	
Total mass flow (kg/h)	1,801.92		1,801.92		6,457.18		1,888.73		8,345.91	
Vapor fraction	0		0		0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.957	0.855	0.957	0.855	1.000	1.000	0.000	0.000	0.884	0.774
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.015	0.095	0.015	0.095	0.000	0.000	0.000	0.000	0.000	0.000
Monochlorohydrins	2.83 E-14	1.55 E-13	2.83 E-14	1.55 E-13	0.000	0.000	0.000	0.000	0.000	0.000
Hexanoic Acid	2.06 E-7	1.18 E-6	2.06 E-7	1.18 E-6	0.000	0.000	0.000	0.000	0.000	0.000
Hydrogen Chloride	0.028	0.050	0.028	0.050	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	1.000	1.000	0.116	0.226
Sodium Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Epichlorohydrin	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Stream	24		25		26	
T (K)	361.97		363.15		363.15	
P (kPa)	100		30		30	
Total molar flow (kmol/h)	494.95		494.95		48.15	
Total mass flow (kg/h)	10,147.83		10,147.83		5,710.80	
Vapor fraction	0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.897	0.784	0.897	0.784	0.093	0.014
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.003	0.017	0.003	0.017	0.907	0.986
Monochlorohydrins	5.10 E-15	2.74 E-14	5.10 E-15	2.74 E-14	0.000	0.000
Hexanoic Acid	3.71 E-8	2.09 E-7	3.71 E-8	2.09 E-7	0.000	0.000
Hydrogen Chloride	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.095	0.185	0.095	0.185	0.000	0.000
Sodium Chloride	0,005	0.014	0,005	0.014	0.000	0.000
Epichlorohydrin	0.000	0.000	0.000	0.000	0.000	0.000

Stream	27		28		29		30		31	
T (K)	363,15		363.15		303.15		363.15		327,02	
P (kPa)	30		30		100		30		30	
Total molar flow (kmol/h)	55.00		91.39		549.67		549.67		91.39	
Total mass flow (kg/h)	990.83		4,357.74		12,491.72		12,491.72		4,357.74	
Vapor fraction	1		1		0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	1.000	1.000	0.602	0.227	0.893	0.704	0.893	0.704	0.602	0.227
Glycerol	0.000	0.000	0.000	0.000	4.28 E-4	0.002	4.28 E-4	0.002	0.000	0.000
Dichlorohydrins	0.000	0.000	0.000	0.000	0.004	0.023	0.004	0.023	0.000	0.000
Monochlorohydrins	0.000	0.000	0.000	0.000	4,59 E-15	2.23 E-14	4,59 E-15	2.23 E-14	0.000	0.000
Hexanoic Acid	0.000	0.000	0.000	0.000	3.34 E-08	1.70 E-07	3.34 E-08	1.70 E-07	0.000	0.000
Hydrogen Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.000	0.000	0.000	0.000	0.009	0.015	0.009	0.015	0.000	0.000
Sodium Chloride	0.000	0.000	0.000	0.000	0.083	0.211	0.083	0.211	0.000	0.000
Epichlorohydrin	0.000	0.000	0.398	0.773	0.011	0.045	0.011	0.045	0.398	0.773

Stream	32		33		34		35		36	
T (K)	327.02		327.02		327.02		389.15		459.69	
P (kPa)	100		100		100		100		450	
Total molar flow (kmol/h)	91.39		52.91		38.48		38.48		38.48	
Total mass flow (kg/h)	4,357.74		998.39		3,359.35		3,359.35		3,359.35	
Vapor fraction	0		0		0		1		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	0.602	0.227	0.988	0.943	0.070	0.015	0.070	0.015	0.070	0.015
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Monochlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hexanoic Acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hydrogen Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Epichlorohydrin	0.398	0.773	0.012	0.057	0.930	0.985	0.930	0.985	0.930	0.985

Stream	37 (desorb 1 h)		38		39		40	
T (K)	298.15		459.69		416.57		303.15	
P (kPa)	100		450		100		100	
Total molar flow (kmol/h)	2.61		35,87		35.87		35.87	
Total mass flow (kg/h)	47.01		3312.34		3312.34		3312.34	
Vapor fraction	1		0		0		0	
	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.	Mole frac.	Mass frac.
Methanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water	1.000	1.000	0.003	0.001	0.003	0.001	0.003	0.001
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dichlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Monochlorohydrins	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hexanoic Acid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hydrogen Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Hydroxide	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Sodium Chloride	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Epichlorohydrin	0.000	0.000	0.997	0.999	0.997	0.999	0.997	0.999