Batch Manufacture of Propylene Glycol

by

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Problem Statement:

Propylene glycol ($C_3H_8O_2$, PG) is produced from propylene oxide (C_3H_6O, PO) by liquid phase hydrolysis with excess water in the presence of a small concentration of sulfuric acid as the catalyst. The reaction is:

$$C_3H_6O + H_2O \xrightarrow{H_2SO_4} C_3H_8O_2$$

The reaction takes place at a reasonable rate at near-ambient temperatures, but the temperature rise can be appreciable in a batch reactor, because the heat of reaction is 36,400 Btu/lbmol of propylene oxide at 68°F. To keep the reaction in the liquid phase, it is important to control the temperature of the reaction mixture, since propylene oxide is a rather low-boiling species (T_{nbp} = 93.7°F). A large excess of water is used for this purpose. In addition, methanol is added to prevent phase splitting because propylene oxide is not completely soluble in water. The resulting liquid mixture is a nonideal solution, which can be modeled adequately with the NRTL equation.

The reaction can be modeled with power-law kinetics that is first order in the propylene oxide concentration, with a rate constant given by:

$$k = Ae^{-E/RT}$$

where the pre-exponential factor, $A = 4.711 \times 10^9 \text{ sec}^{-1}$, and the activation energy, E = 32,400 Btu/lbmol.

To manufacture one batch of propylene glycol, the following recipe is proposed:

1. Charge a mixture of 43.04 lbmol of propylene oxide, 802.8 lbmol of water and 71.87 lbmol of methanol, at 77°F, to the reactor over 30 min. The reactor volume is 400 ft^3 (D = 8.0 ft, H = 8.0 ft, aspect ratio = 1, which minimizes the purchase

cost). Start the reaction by adding 0.1 wt % (20 lb) of sulfuric acid in 1 min to the mixture and allow the mixture to react for 30 min.

2. Add 0.4078 lbmol (16.3 lb) of sodium hydroxide in 1 min to quench the reaction and neutralize the catalyst. Allocate 10 min for the neutralization reaction. Then, transfer the neutralized effluent to the distillation still in 10 min.

3. Recover the propylene glycol by using a 15-tray batch distillation operation with a total condenser:

   a. Bring the column to total reflux over 1 hr.

   b. Using a reflux ratio of 5, send 200 lbmol/hr of distillate continuously to the reflux accumulator, until the mole fraction of propylene glycol in the instantaneous distillate reaches 0.01. The tray and condenser liquid holdups are 0.3 ft^3/tray and 3.0 ft^3, respectively. The still tank has the same dimensions as the reactor.

   c. Transfer the contents of the distillation still to the PG accumulator over 10 min.

   Assume that the pressure in the column is 1 atm and there is no pressure drop on each stage. The water and methanol are collected in the distillate product accumulator so that the mixture can be recycled to the reactor.

(a) Use BATCH PLUS to simulate the production of one batch of propylene glycol and determine the batch cycle time, using the above specifications. Have BATCH PLUS prepare a 3-batch Gantt chart.

(b) Determine the selling price of propylene glycol to achieve a 20% rate of return on investment. Let the price of propylene oxide be $0.72/lb. Assume the costs of site preparation, service facilities, land, royalties, and startup are negligible. Let the cost of contingencies and contractor's fee be 18% of the direct permanent investment. Provide for working capital to cover 2 days of raw material inventory, 2 days of finished product inventory, and 30 days of accounts receivable.

(c) Repeat (b) using two batch distillation towers in parallel.

Solution – Part (a):

The text recipe for the BATCH PLUS simulation of the process is:

```
----------------------------------------------------------------------
1.    Reaction
1.1.  Charge Reactor Tank with 71.87 lbmole of METHANOL. The charge
      time is 30 min. Charge Reactor Tank with 43.04 lbmole of
      PROPYLENE-OXIDE. The charge time is 30 min. Charge Reactor Tank
      with 802.8 lbmole of WATER. The charge time is 30 min.
1.2.  Charge Reactor Tank with 20 lb of SULFURIC-ACID. The charge time
      is 1 min.
1.3.  React in unit Reactor Tank via Main Reaction. The reaction
      mixture is Liquid-Only. Stop when operation time reaches 30 min.

----------------------------------------------------------------------
2.    Neutralization
2.1.  Charge Reactor Tank with 0.4078 lbmole of SODIUM-HYDROXIDE. The
      charge time is 1 min. Dissolve 100%  of all solids.
2.2.  React in unit Reactor Tank via Neutralization Reaction. The
      reaction is Adiabatic. Reaction occurs over 10 min.
2.3.  Transfer contents of unit Reactor Tank to Distillation Still.
      Transfer 100% of vessel contents. The transfer time is 10 min.

----------------------------------------------------------------------
3.    Distillation
3.1.  Distill the batch in unit Distillation Still.  The overhead is
      sent to MW Accumulator. The column has 15 equilibrium stages. The
      operation type is distill with total reflux (TRFLX-ALSO). The
      condenser is a total condenser  (TOTAL). The reflux ratio is 5 on
      a mole basis. The average distillate rate is 0.055556 lbmole/s.
      Time for total reflux operation is 1 h. The boilup rate for total
      reflux is 0.27778 lbmole/s. The condenser pressure is 14.7 psi.
      The pressure drop for each stage is 0 psi. The condenser holdup
      is 3 Cubic ft. The holdup on each stage is 0.3 Cubic ft. Distill
      until Mole fraction of PROPANEDIOL-1,2 reaches 0.01 in the
      accumulator from below. If stop condition is not reached end
      after 120 h of operation time.
3.2.  Transfer contents of unit Distillation Still to PG Accumulator.
      Transfer 100% of vessel contents. The transfer time is 10 min.
```

The equipment contents report for the reactor tank follows:

Step Equipment Contents

Process (Version)	PG Manufacture (1.0)	**Key Input Intermediate:**	PROPYLENE-OXIDE
Step (Version):	PG Manufacture (1.0)	**Key Output Intermediate:**	PROPANEDIOL-1,2
Simulation Date:	6/21/2004 10:52	**Number of Batches:**	1
		Plan Quantity:	2,635.83 lb

Reactor Tank

Operation		START	1.1. Charge	1.2. Charge	1.3. React	2.1. Charge	2.2. React
Time	**(min)**	0.00	30.00	31.00	61.00	62.00	72.00
Mole - (lbmole)	**Mol Wt**						
Total		1.0309	917.9026	918.1061	875.0255	875.4330	875.4317
METHANOL	32.04		71.8700	71.8700	71.8700	71.8700	71.8700
PROPYLENE-OXIDE	58.08		43.0400	43.0400	0.0000	0.0000	0.0000
PROPANEDIOL-1,2	76.10				43.0399	43.0399	43.0399
SODIUM-HYDROXIDE	40.00					0.4078	
WATER	18.02		802.8000	802.8000	759.7601	759.7601	760.1679
SULFURIC-ACID	98.08			0.2039	0.2039	0.2039	0.0000
NITROGEN	28.01	0.8144	0.1522	0.1518	0.1197	0.1194	0.1184
SODIUM-SULFATE	142.00						0.2039
OXYGEN	32.00	0.2165	0.0405	0.0404	0.0318	0.0318	0.0315
Liquid+Solid Mass	**(lb)**	0.00	19,268.93	19,288.93	19,288.93	19,305.25	19,305.24
Liquid+Solid Volume	**(Cubic ft)**	0.00	328.51	328.68	334.89	335.02	335.41
Phase		Gas	Gas+Liquid1	Gas+Liquid1	Gas+Liquid1	Gas+Liquid1	Gas+Liquid1
Temperature	**(F)**	77.00	77.00	77.00	165.14	165.11	167.04
Pressure	**(psi)**	14.70	14.70	14.70	14.70	14.70	14.70
Average Liq+Sol Density	**(lb/Cubic ft)**	0.00	58.66	58.69	57.60	57.62	57.56
Average Liq+Sol Viscosity	**(cp)**	0.00	0.79	0.81	1.14	1.52	1.11
Average Liq+Sol Heat Capacity	**(BTU/lb-R)**	0.00	0.89	0.89	0.91	0.91	0.91
Average Liq+Sol Molecular Weight		0.00	21.00	21.01	22.05	22.06	22.06

As can be seen in the equipment contents report, all of the propylene oxide has reacted after 30 min, forming 43.04 lbmol of propylene glycol. The temperature rise is significant (from 77°F to 165°F), and consequently, the possible vaporization of propylene oxide during the reaction is a concern. However, as shown in Figure 1, during the reaction, the bubble point temperature at each conversion is always significantly higher (>30°F) than the temperature of the reaction mixture. Therefore, the vaporization of propylene oxide is minimal and no cooling is required.

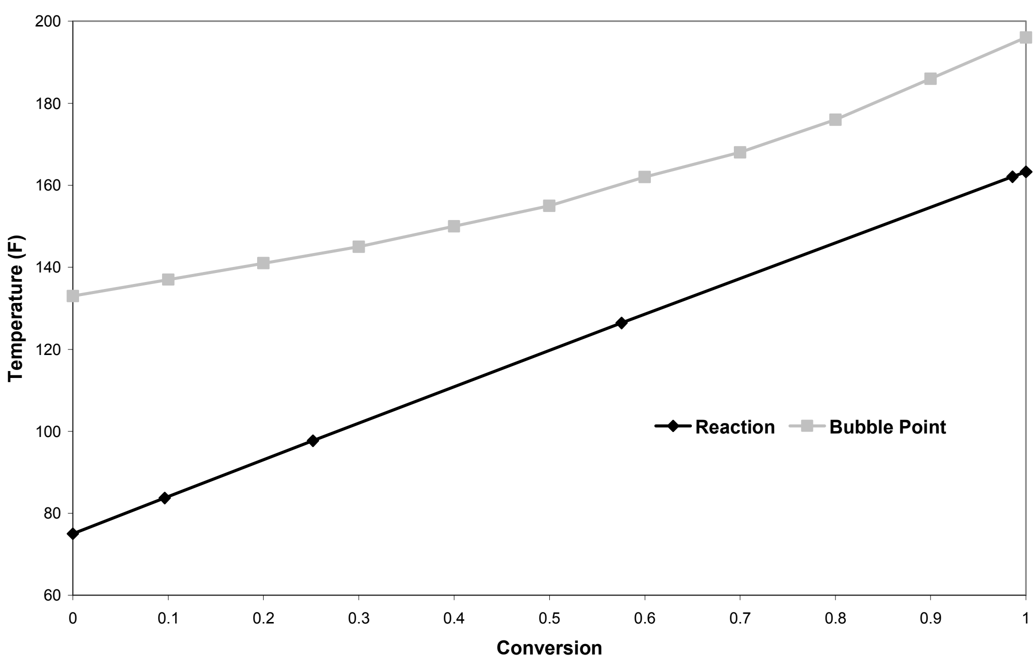


Figure 1 Reactor temperature as function of conversion

After 30 min of reaction time, caustic (sodium hydroxide) is added to neutralize the sulfuric acid and quench the reaction. Although the neutralization reaction is highly exothermic, the low concentration of sulfuric acid keeps the temperature rise at only 2°F.

After the mixture has been neutralized, it is transferred to the still tank to be distilled. As specified, the light species (methanol and water) are collected in one accumulator (MW) and the product (propylene glycol) is collected in another (PG). The equipment contents reports for the two accumulators are:

Step Equipment Contents

Process (Version) PG Manufacture (1.0)
Step (Version): PG Manufacture (1.0)
Simulation Date: 6/21/2004 10:52

Key Input Intermediate: PROPYLENE-OXIDE
Key Output Intermediate: PROPANEDIOL-1,2
Number of Batches: 1
Plan Quantity: 2,635.83 lb

MW Accumulator

Operation		START	3.1. Distill	3.1. Distill
Time	(min)	0.00	82.00	394.10
Mole - (lbmole)	Mol Wt			
☑ Total		1.0309	1.0309	840.4696
METHANOL	32.04			71.8709
PROPYLENE-OXIDE	58.08			0.0000
PROPANEDIOL-1,2	76.10			8.4035
WATER	18.02			760.0801
NITROGEN	28.01	0.8144	0.8144	0.0909
OXYGEN	32.00	0.2165	0.2165	0.0242
Liquid+Solid Mass	(lb)	0.00	0.00	16,638.90
Liquid+Solid Volume	(Cubic ft)	0.00	0.00	336.14
Phase		Gas	Gas	Gas+Liquid1
Temperature	(F)	77.00	77.00	347.87
Pressure	(psi)	14.70	14.70	14.70
Average Liq+Sol Density	(lb/Cubic ft)	0.00	0.00	49.50
Average Liq+Sol Viscosity	(cp)	0.00	0.00	0.21
Average Liq+Sol Heat Capacity	(BTU/lb-R)	0.00	0.00	1.02
Average Liq+Sol Molecular Weight		0.00	0.00	19.80

Step Equipment Contents

Process (Version) PG Manufacture (1.0)
Step (Version): PG Manufacture (1.0)
Simulation Date: 6/21/2004 10:52

Key Input Intermediate: PROPYLENE-OXIDE
Key Output Intermediate: PROPANEDIOL-1,2
Number of Batches: 1
Plan Quantity: 2,635.83 lb

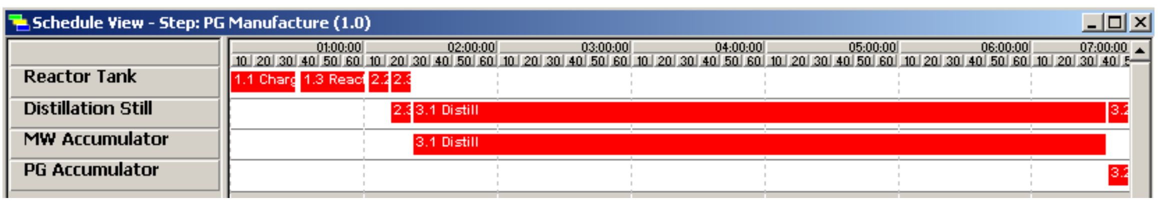
PG Accumulator

Operation		START	3.2. Transfer	3.2. Transfer
Time	(min)	0.00	394.10	404.10
Mole Fraction	Mol Wt			
☑ Total		1.0000	1.0000	1.0000
PROPANEDIOL-1,2	76.10			0.9910
WATER	18.02			0.0025
SULFURIC-ACID	98.08			0.0000
NITROGEN	28.01	0.7900	0.7900	0.0005
SODIUM-SULFATE	142.00			0.0058
OXYGEN	32.00	0.2100	0.2100	0.0001
Liquid+Solid Mass	(lb)	0.00	0.00	2,666.37
Liquid+Solid Volume	(Cubic ft)	0.00	0.00	49.94
Phase		Gas	Gas	Gas+Liquid1
Temperature	(F)	77.00	77.00	423.75
Pressure	(psi)	14.70	14.70	14.70
Average Liq+Sol Density	(lb/Cubic ft)	0.00	0.00	53.40
Average Liq+Sol Viscosity	(cp)	0.00	0.00	1.93
Average Liq+Sol Heat Capacity	(BTU/lb-R)	0.00	0.00	0.86
Average Liq+Sol Molecular Weight		0.00	0.00	76.34

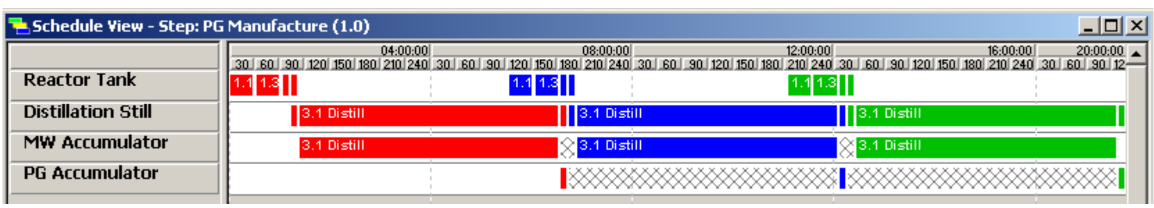
The MW accumulator contents report shows that distillation occurs from 82 to 394 min. During the first hour, total reflux is achieved (not shown). Then the MW product is accumulated over 4 hr 12 min. The PG accumulator contents report shows that, at this time, the purity of the propylene glycol product is 99%. Unfortunately, to achieve this high purity, 8.4 lbmol of propylene glycol are lost with the methanol and water product. The methanol and water are recycled to be used in another batch, with makeup water added to replace that consumed in the reaction.

The schedule view (Gantt chart) of the simulation shows the time required for each operation. The whole process takes nearly 7 hr, and the batch cycle time is 5 hr and 32 min. Assuming the process is operational 330 day/yr, there are 1,431 batches/yr.

The distillation step requires over 4 hr and is the longest step in the process. This is due to the large amount of water removed. The batch time for this step can be shortened by increasing the distillate rate. In so doing, however, the product purity is reduced (more PG is lost) and the utility costs are increased.



a. Schedule view for a single batch



b. Schedule view for 3 batches

Figure 2 Gantt charts

Solution – Part (b):

To estimate the selling price of propylene glycol for the batch process, estimates for the cost of production and the total capital investment are necessary. Next, equipment sizes and costs are estimated using the techniques in Chapters 13-16, SSL.

Distillation Column

D = 2.4 ft (determined from Eq. (14.11))
Holdup = 0.3 ft^3 (weir height ~ 1 inch)
Number of trays = 15
Tray spacing = 2 ft

Since this is a batch distillation operation, the feed is charged into the still tank, which serves as the reboiler, as shown in Figure 2. Hence, 10 ft are not allocated at the bottom of the column with only 2 ft needed. The height of the column section is:

$$H = 4 + (15 - 1) \times 2 + 2 = 34 \text{ ft}$$

Adjusting Eq. (16.59), since the lower head is not included, the weight of the shell and 1 head is:

W = 2,714 lb
$C_{V,column}$ = \$20,300
C_{PL} = \$7,000

Using Eqs. (16.66) – (16.68), for 15 sieve trays, C_T = \$10,300

Total purchase cost = $C_{P,tower}$ = \$37,500

Using Table 16.11 to obtain the bare module factor:

F_{BM} = 4.16
C_{BM} = \$156,100

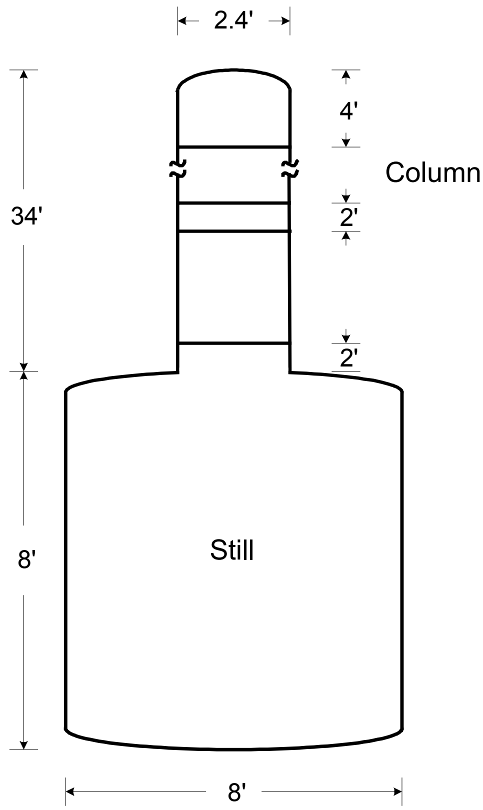


Figure 2 Batch distillation column

Reflux Accumulator

Horizontal Vessel (residence time = 5 min, half full):

Aspect Ratio = 2
$D = 2.6$ ft
$L = 5.2$ ft
$C_P = \$10{,}000$
$F_{BM} = 3.05$
$C_{BM} = \$30{,}700$

Condenser

$Q = 2.86 \times 10^7$ Btu/hr (average cooling load determined by BATCH PLUS)

The largest area is required at the smallest ΔT_{LM}; that is, when nearly pure methanol is recovered. Note that the normal boiling point of methanol is 150°F. Assuming that cooling water enters at 90°F and exits at 120°F:

$$\Delta T_{LM} = \frac{(150-90)-(150-120)}{\ln\left(\dfrac{150-90}{150-120}\right)} = 43^\circ \text{F}$$

Using Table 13.5, a conservative assumption for the overall heat transfer coefficient is $U = 100 \dfrac{\text{Btu}}{\text{ft}^2 \cdot \text{hr} \cdot \text{F}}$. Substituting in Eq. (13.2):

$$A = \frac{Q}{U\Delta T_{LM}} = 6{,}651 \text{ ft}^2$$

For a fixed head, carbon steel heat exchanger:

C_P = \$38,000
F_{BM} = 3.17
C_{BM} = \$121,300

Reboiler

$Q = 2.86 \times 10^7$ Btu/hr (average heating load determined by BATCH PLUS)

Assuming a heat flux of 12,000 Btu/hr-ft^2 to avoid film boiling:

A = 2,400 ft^2

A kettle reboiler, carbon steel heat exchanger is used with:

C_P = \$41,100
F_{BM} = 3.17
C_{BM} = \$130,300

Reflux Pump

Power = 0.37 Hp (change in pressure = 17.3 psi)
Volumetric flow rate = 36 gal/min
Pump head = 40 ft

Using a single-stage pump with shaft rotation of 3,600 rpm, VSC case split, cast steel:

C_P = \$2,600

Cost of an explosion proof motor:

$C_{P,motor}$ = \$400

Total purchase cost = \$3,000
F_{BM} = 3.3
C_{BM} = \$10,000

Distillation Still

Using a vertical pressure vessel of diameter 8 ft and aspect ratio of 1:

From Eq. (16.59), weight of the shell and 2 heads is:

W = 5,563 lb
C_P = \$29,000

F_{BM} = 4.16
C_{BM} = \$121,000

Reactor Tank

Same dimensions as Distillation Still, but stainless steel-304 is used to prevent corrosion:

C_{BM} = \$189,000

Propylene Oxide Storage Tank

Storage is provided for a two-day supply of propylene oxide.

Batch cycle time = 5 hr 32 min
Number of batches run in 2 days = 9

Volume of one batch of propylene oxide

$$= 43.04\ \text{lbmol} \times \frac{58.08\ \text{lb}}{\text{lbmol}} \times \frac{\text{ft}^3}{0.833 \times 62.4\text{lb}}$$

$= 48\ \text{ft}^3$

Using a vertical vessel with a diameter of 8.5 ft and an aspect ratio of 1 (volume = 482 ft^3):

W = 6,279 lb
C_P = \$31,300
F_{BM} = 4.16
C_{BM} = \$130,300

Methanol and Water Collector

The methanol and water collector acts as a surge tank to allow 2 days of methanol and water inventory.

Volume of one batch of methanol and water = 336 ft^3
Number of batches run in 2 days = 9

Using a vertical vessel with a diameter of 16.5 ft and an aspect ratio of 1 (volume = 3,500 ft^3):

W = 23,600 lb
C_P = \$73,000
F_{BM} = 4.16
C_{BM} = \$303,500

Propylene Glycol Collector

The propylene glycol collector acts as a storage tank to allow 2 days of propylene glycol inventory.

Volume of propylene glycol in one batch = 50 ft^3
Number of batches run in 2 days = 9

Using a vertical pressure vessel of diameter 8.75 ft and aspect ratio of 1 (volume = 530 ft^3):

W = 6,653 lb
C_P = \$32,500
F_{BM} = 4.16
C_{BM} = \$135,100

Selling Cost Calculation

Utility Cost

When calculating the cost of this campaign, the utility costs and the material costs are considered. The total reboiler heat duty computed by BATCH PLUS is 1.49×10^8 Btu. The maximum bottoms temperature is 369°F, the normal boiling point of propylene glycol. Because the saturation temperature of medium-pressure steam (150 psig) is 365°F, high-pressure steam (450 psig) is used to heat the reboiler. An overall temperature driving force of 41°F is used to insure film boiling, which reduces the steam condensation temperature to 369 + 41 = 410°F. The latent heat of vaporization of steam at 410°F is 816 Btu/lb. The cost of steam is therefore:

$$\frac{1.49 \times 10^8 \text{ Btu}}{816 \text{ Btu/lb}} \times \frac{\$5.50}{1{,}000 \text{ lb}} = \$1{,}004 / \text{batch}$$

The total condenser heat duty is 1.49×10^8 Btu. Cooling water is used in the condenser. It is assumed that the cooling water enters at 90°F and exits at 120°F. The specific heat of water is 1 Btu/lb°F, and the density is 8.33 lb/gal. The cost of cooling water is therefore:

$$\frac{1.49 \times 10^8 \text{ Btu}}{\left(1 \frac{\text{Btu}}{\text{lb°F}}\right)(30\text{°F})} \times \frac{\text{gal}}{8.33 \text{ lb}} \times \frac{\$0.05}{1{,}000 \text{ gal}} = \$29.81 / \text{batch}$$

Total utility cost = $1,034/batch

Raw Materials Cost

Only the raw materials cost of propylene oxide is considered, since methanol is recycled, and the amount of makeup water is small:

Price of propylene oxide = $0.72/lb
Total amount of PO needed = 2,500 lb/batch
Total raw materials cost = $1,800/batch

Installed Equipment Cost

Equipment	Cost
Column + Trays	156,100
Reflux Accumulator	30,700
Condenser	121,300
Reboiler	130,300
Reflux Pump	10,000
Reactor Tank	189,000
Distillation Still	121,000
PO Storage Tank	130,300
MW Collector	303,500
PG Collector	135,100
Total Bare Module Cost	$1,327,300

Total Capital Investment

C_{TBM} = $1,327,300

Ignoring costs of site preparation and service facilities, the direct permanent investment is:

C_{DPI} = $1,327,300

and the cost of contingencies and contractor fees is:

$C_{cont} = 0.18\,C_{DPI}$ = $238,900

Adding, the total depreciable capital is:

C_{TDC} = $1,566,000

Ignoring costs of land, royalties and plant startup, the total permanent investment is:

C_{TPI} = $1,566,000

Working capital, C_{WC}:

Number of batches in 30 days = 130
Price of propylene glycol = $$X$/lb
Accounts receivable = (130 batches)(2,636 lb/batch)($$X$/lb) = $342,700$X$

Number of batches in 2 days = 9
Price of propylene oxide = $0.72/lb
Total amount of PO needed = 2,500 lb/batch
2 day raw material inventory = (9 batches) (2,500 lb/batch)($0.72/lb) = $16,200

C_{WC} = \$16,200 + \$342,700X

Adding the working capital to the total permanent investment, gives the total capital investment:

C_{TCI} = \$1,582,200 + \$342,700X

Total Annual Production Cost

C = (\$1,800 + \$1,034)*1,431 = \$4,055,000

Price of propylene glycol = \$$X$/lb
Total mass of PG produced = 2,636 lb/batch
Total sales = \$2,636X/batch
Total annual sales:

S = \$2,636X *1,431 = \$3,772,000X

Propylene Glycol Selling Price

Rate of return on investment $= 0.2 = \frac{(1-t)(S-C)}{C_{\text{TCI}}} = \frac{(1-0.37)(3{,}772{,}000X - 4{,}055{,}000)}{1{,}582{,}200 + 342{,}700X}$

Solving for X, X = \$1.25/lb

To achieve a 20% rate of return on investment, the selling price of propylene glycol must be at least \$1.25/lb. The minimum selling price under continuous operation is expected to be lower, since economies of scale can be achieved with larger equipment and higher throughput. Batch operation is inefficient when dealing with large quantities. Note that the *Chemical Market Reporter* gives a price of \$0.72/lb for purchase of commodity quantities of propylene oxide.

Solution – Part(c) - Parallel Distillation Units

To shorten the batch cycle time, the reactor effluent stream is halved and purified in two parallel distillation units. The text recipe for this design is:

```
----------------------------------------------------------------------
1.     Reaction
1.1.   Charge Reactor Tank with 71.87 lbmole of METHANOL. The charge
       time is 30 min. Charge Reactor Tank with 43.04 lbmole of
       PROPYLENE-OXIDE. The charge time is 30 min. Charge Reactor Tank
       with 802.8 lbmole of WATER. The charge time is 30 min.
1.2.   Charge Reactor Tank with 20 lb of SULFURIC-ACID. The charge time
       is 1 min.
1.3.   React in unit Reactor Tank via Main Reaction. The reaction
       mixture is Liquid-Only. Stop when operation time reaches 30 min.

----------------------------------------------------------------------
2.     Neutralization
2.1.   Charge Reactor Tank with 0.4078 lbmole of SODIUM-HYDROXIDE. The
       charge time is 1 min. Dissolve 100% of all solids.
2.2.   React in unit Reactor Tank via Neutralization Reaction. The
       reaction is Adiabatic. Reaction occurs over 10 min.

----------------------------------------------------------------------
3.     Distillation
3.1.   Transfer contents of unit Reactor Tank to Distillation Still 1.
       Transfer 50% of vessel contents. The transfer time is 10 min.
       Start Parallel
             Series
3.2.         Distill the batch in unit Distillation Still 1. The
             overhead is sent to MW Accumulator 1. The column has 15
             equilibrium stages. The operation type is distill with
             total reflux (TRFLX-ALSO). The condenser is a total
             condenser (TOTAL). The reflux ratio is 5 on a mole basis.
             The average distillate rate is 0.055556 lbmole/s. Time for
             total reflux operation is 1 h. The boilup rate for total
             reflux is 0.27778 lbmole/s. The condenser pressure is 14.7
             psi. The pressure drop for each stage is 0 psi. The
             condenser holdup is 1.5 Cubic ft. The holdup on each stage
             is 0.15 Cubic ft. Distill until Mole fraction of
             PROPANEDIOL-1,2 reaches 0.01 in the accumulator from below.
             If stop condition is not reached end after 120 h of
             operation time.
3.3.         Transfer contents of unit Distillation Still 1 to PG
             Accumulator. Transfer 100% of vessel contents. The transfer
             time is 10 min.
             Series
3.4.         Transfer contents of unit Reactor Tank to Distillation
             Still 2. Transfer 100% of vessel contents. The transfer
             time is 10 min.
3.5.         Distill the batch in unit Distillation Still 2. The
             overhead is sent to MW Accumulator 2. The column has 15
             equilibrium stages. The operation type is distill with
             total reflux (TRFLX-ALSO). The condenser is a total
             condenser (TOTAL). The reflux ratio is 5 on a mole basis.
             The average distillate rate is 0.055556 lbmole/s. Time for
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             total reflux operation is 1 h. The boilup rate for total
             reflux is 0.27778 lbmole/s. The condenser pressure is 14.7
             psi. The pressure drop for each stage is 0 psi. The
             condenser holdup is 1.5 Cubic ft. The holdup on each stage
             is 0.15 Cubic ft. Distill until Mole fraction of
             PROPANEDIOL-1,2 reaches 0.01 in the accumulator from below.
             If stop condition is not reached end after 120 h of
             operation time.
3.6.         Transfer contents of unit Distillation Still 2 to PG
             Accumulator. Transfer 100% of vessel contents. The transfer
             time is 10 min.
      End Parallel
```

Note that the specifications for distillation (distillate rate, holdups, stop conditions) have been adjusted to maintain the purity of the propylene glycol at 99%. The equipment contents report for the accumulators is:

Step Equipment Contents

Process (Version)	PG Manufacture (1.0)	**Key Input Intermediate:**	PROPYLENE-OXIDE
Step (Version):	PG Manufacture (1.0)	**Key Output Intermediate:**	PROPANEDIOL-1,2
Simulation Date:	6/21/2004 15:53	**Number of Batches:**	1
		Plan Quantity:	2,635.83 lb

PG Accumulator

Operation		START	3.3. Transfer	3.3. Transfer	3.6. Transfer	3.6. Transfer
Time	**(min)**	0.00	268.05	278.05	278.05	288.05
Mole Fraction	**Mol Wt**					
Total		1.0000	1.0000	1.0000	1.0000	1.0000
METHANOL	32.04			0.0000	0.0000	0.0000
PROPANEDIOL-1,2	76.10			0.9876	0.9876	0.9907
WATER	18.02			0.0025	0.0025	0.0025
SULFURIC-ACID	98.08			0.0000	0.0000	0.0000
NITROGEN	28.01	0.7900	0.7900	0.0032	0.0032	0.0008
SODIUM-SULFATE	142.00			0.0058	0.0058	0.0058
OXYGEN	32.00	0.2100	0.2100	0.0008	0.0008	0.0002
Liquid+Solid Mass	**(lb)**	0.00	0.00	1,333.20	1,333.20	2,666.36
Liquid+Solid Volume	**(Cubic ft)**	0.00	0.00	24.96	24.96	48.88
Phase		Gas	Gas	Gas+Liquid1	Gas+Liquid1	Gas+Liquid1
Temperature	**(F)**	77.00	77.00	423.41	423.41	396.61
Pressure	**(psi)**	14.70	14.70	14.70	14.70	14.70
Average Liq+Sol Density	**(lb/Cubic ft)**	0.00	0.00	53.41	53.41	54.55
Average Liq+Sol Viscosity	**(cp)**	0.00	0.00	1.93	1.93	1.73
Average Liq+Sol Heat Capacity	**(BTU/lb-R)**	0.00	0.00	0.86	0.86	0.84
Average Liq+Sol Molecular Weight		0.00	0.00	76.34	76.34	76.34

Step Equipment Contents

Process (Version)	PG Manufacture (1.0)	**Key Input Intermediate:**	PROPYLENE-OXIDE
Step (Version):	PG Manufacture (1.0)	**Key Output Intermediate:**	PROPANEDIOL-1,2
Simulation Date:	6/21/2004 15:53	**Number of Batches:**	1
		Plan Quantity:	2,635.83 lb

MW Accumulator 1

Operation		START	3.2. Distill	3.2. Distill
Time	**(min)**	0.00	82.00	268.05
Mole - (lbmole)	**Mol Wt**			
Total		0.5103	0.5103	420.2306
METHANOL	32.04			35.9349
PROPYLENE-OXIDE	58.08			0.0000
PROPANEDIOL-1,2	76.10			4.2018
WATER	18.02			380.0397
NITROGEN	28.01	0.4032	0.4032	0.0429
OXYGEN	32.00	0.1072	0.1072	0.0114
Liquid+Solid Mass	**(lb)**	0.00	0.00	8,319.42
Liquid+Solid Volume	**(Cubic ft)**	0.00	0.00	168.01
Phase		Gas	Gas	Gas+Liquid1
Temperature	**(F)**	77.00	77.00	347.47
Pressure	**(psi)**	14.70	14.70	14.70
Average Liq+Sol Density	**(lb/Cubic ft)**	0.00	0.00	49.52
Average Liq+Sol Viscosity	**(cp)**	0.00	0.00	0.21
Average Liq+Sol Heat Capacity	**(BTU/lb-R)**	0.00	0.00	1.02
Average Liq+Sol Molecular Weight		0.00	0.00	19.80

Step Equipment Contents

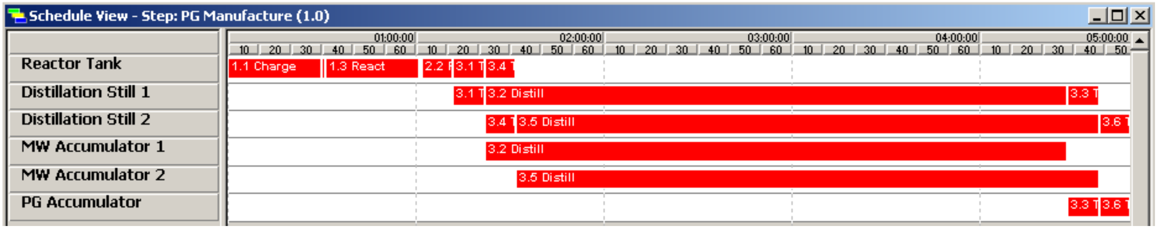
Process (Version)	PG Manufacture (1.0)	**Key Input Intermediate:**	PROPYLENE-OXIDE
Step (Version):	PG Manufacture (1.0)	**Key Output Intermediate:**	PROPANEDIOL-1,2
Simulation Date:	6/21/2004 15:53	**Number of Batches:**	1
		Plan Quantity:	2,635.83 lb

MW Accumulator 2

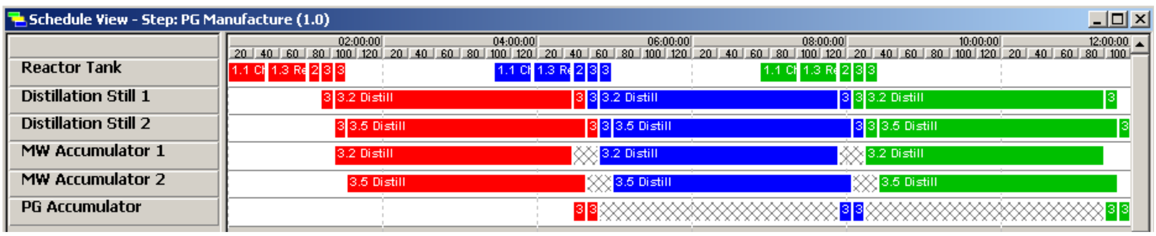
Operation		START	3.5. Distill	3.5. Distill
Time	**(min)**	0.00	92.00	278.05
Mole - (lbmole)	**Mol Wt**			
Total		0.5103	0.5103	420.2323
METHANOL	32.04			35.9354
PROPYLENE-OXIDE	58.08			0.0000
PROPANEDIOL-1,2	76.10			4.2018
WATER	18.02			380.0410
NITROGEN	28.01	0.4032	0.4032	0.0427
OXYGEN	32.00	0.1072	0.1072	0.0114
Liquid+Solid Mass	**(lb)**	0.00	0.00	8,319.47
Liquid+Solid Volume	**(Cubic ft)**	0.00	0.00	168.12
Phase		Gas	Gas	Gas+Liquid1
Temperature	**(F)**	77.00	77.00	348.14
Pressure	**(psi)**	14.70	14.70	14.70
Average Liq+Sol Density	**(lb/Cubic ft)**	0.00	0.00	49.49
Average Liq+Sol Viscosity	**(cp)**	0.00	0.00	0.21
Average Liq+Sol Heat Capacity	**(BTU/lb-R)**	0.00	0.00	1.02
Average Liq+Sol Molecular Weight		0.00	0.00	19.80

As shown, the purity of the propylene glycol product is maintained at 99%. The amount of propylene glycol produced in each batch is also the same. The batch time (3 hr 26 min) is shorter than for a single distillation column (5 hr 32 min). As a result, more batches are run annually. Assuming the process operates 330 day/yr, the number of batches per year is 2,306.

The schedule view for a single batch is:



The schedule view for three batches is:



Distillation Column

D = 1.9 ft (determined using Eq. (14.11))
Holdup = 0.15 ft^3 (weir height ~ 1 inch)
Number of trays = 15
Tray spacing = 2 ft
$H = 4 + (15-1)\times 2 + 2 = 34$ ft

Adjusting Eq. (16.59), the weight of the shell and 1 head is:

W = 2,141 lb
$C_{V,\text{column}}$ = \$17,800
C_{PL} = \$6000

For 15 sieve trays, C_T = \$9,400

Total purchase cost = $C_{P,\text{tower}}$ = \$33,200
F_{BM} = 4.16
C_{BM} = \$138,400

Reflux Accumulator

Horizontal Vessel (residence time = 5 min, half full):

Aspect Ratio = 2
$D = 2$ ft
$L = 4$ ft
C_P = \$8,800
$F_{BM} = 3.05$
C_{BM} = \$26,800

Condenser

$Q = 2.88 \times 10^7$ Btu/hr (average cooling load determined by BATCH PLUS)

The largest area is required at the smallest ΔT_{LM}; that is, when nearly pure methanol is recovered. Note that the normal boiling point of methanol is 150°F. Assuming that cooling water enters at 90°F and exits at 120°F,

$$\Delta T_{LM} = \frac{(150-90)-(150-120)}{\ln\left(\frac{150-90}{150-120}\right)} = 43^\circ \text{F}$$

Assuming $U = 100 \frac{\text{Btu}}{\text{ft}^2 \cdot \text{hr} \cdot \text{F}}$. Substituting in Eq. (13.2):

$$A = \frac{Q}{U\Delta T_{LM}} = 6{,}667 \text{ ft}^2$$

A fixed head, carbon steel heat exchanger is used with:

C_P = \$38,300
$F_{BM} = 3.17$
C_{BM} = \$121,500

Reboiler

$Q = 2.87 \times 10^7$ Btu/hr (average heating load determined by BATCH PLUS)

Assuming a heat flux of 12,000 Btu/hr-ft^2 to avoid film boiling:

$A = 2{,}392$ ft^2

A kettle reboiler, carbon steel heat exchanger is used with:

C_P = \$41,000
F_{BM} = 3.17
C_{BM} = \$130,100

Reflux Pump

Power = 0.18 Hp (change in pressure = 17.3 psi)
Volumetric flow rate = 18 gal/min
Pump head = 40 ft

Using a single stage pump with shaft rotation of 3,600 rpm, VSC case split, cast steel,

C_P = \$2,700

Cost of an explosion proof motor:

C_P = \$420

Total purchase cost = $C_{P,total}$ = \$3,100
F_{BM} = 3.3
C_{BM} = \$10,400

Reactor Tank

Same as in base case design:

C_{BM} = \$189,000

Distillation Still

Using a vertical pressure vessel of diameter 6.5 ft and aspect ratio of 1 (volume = 216 ft^3).

From Eq. (16.59), weight of the shell and 2 heads is:

W = 3,676 lb
C_P = \$22,700

F_{BM} = 4.16
C_{BM} = \$94,400

Propylene Oxide Storage Tank

Storage is provided for a two-day supply of propylene oxide.

Batch cycle time = 3 hr 26 min
Number of batches run in 2 days = 14

Volume of one batch of propylene oxide = 48 ft^3

Using a vertical vessel with a diameter of 10 ft and an aspect ratio of 1 (volume = 785 ft^3):

W = 8,686 lb
C_P = \$38,300
F_{BM} = 4.16
C_{BM} = \$159,300

Methanol and Water Collector

The methanol and water collector acts as a surge tank to allow 2 days of methanol and water inventory.

Volume of one batch of methanol and water = 336 ft^3
Number of batches run in 2 days = 14

Using a vertical vessel with a diameter of 19 ft and aspect ratio of 1 (volume = 5,400 ft^3):

W = 31,310 lb
C_P = \$88,100
F_{BM} = 4.16
C_{BM} = \$366,400

Propylene Glycol Collector

The propylene glycol collector acts as a storage tank to allow 2 days of inventory.

Volume of propylene glycol in one batch = 50 ft^3
Number of batches run in 2 days = 14

Using a vertical vessel with a diameter of 10 ft and an aspect ratio of 1 (volume = 785 ft^3):

W = 8,686 lb
C_P = \$38,300
F_{BM} = 4.16
C_{BM} = \$159,300

Selling Cost Calculation – Parallel Distillation Units

Utility Cost

The total heat duty for each reboiler computed by BATCH PLUS is 8.92×10^{7} Btu. The maximum bottoms temperature is 369°F, the normal boiling point of propylene glycol. Because the saturation temperature of medium pressure steam (150 psig) is 365°F, high pressure steam (450 psig) is used to heat the reboiler. An overall temperature driving force of 41°F is used to insure film boiling, which reduces the steam condensation temperature to 369 + 41 = 410°F. The latent heat of vaporization of steam at 410°F is 816 Btu/lb. The cost of steam is therefore:

$$\frac{8.92\times10^{7}\,\text{Btu}\times2}{816\,\text{Btu/lb}}\times\frac{\$5.50}{1{,}000\,\text{lb}}=\$1{,}202\,/\,\text{batch}$$

The heat duty for each condenser is 8.9×10^{7} Btu. Cooling water is used at the condensers. It is assumed that the cooling water enters at 90°F and exits at 120°F. The specific heat of water is 1Btu/lb°F, and the density is 8.33 lb/gal. The cost of cooling water is therefore:

$$\frac{8.9\times10^{7}\,\text{Btu}\times2}{\left(1\dfrac{\text{Btu}}{\text{lb°F}}\right)(30\text{°F})}\times\frac{\text{gal}}{8.33\,\text{lb}}\times\frac{\$0.05}{1{,}000\,\text{gal}}=\$35.61\,/\,\text{batch}$$

Total utility cost = $1,238/batch

Raw Materials Cost

Only the raw materials cost of propylene oxide is considered, since methanol is recycled, and the amount of makeup water is small:

Price of propylene oxide = $0.72 / lb
Total amount of PO needed = 2,500 lb
Total raw materials cost = $1,800 / batch

Installed Equipment Cost

Equipment	Cost
Column + Trays (x 2)	276,800
Reflux Accumulator (x 2)	53,600
Condenser (x 2)	243,000
Reboiler (x 2)	260,100
Reflux Pump (x 2)	20,800
Reactor Tank	189,000
Distillation Still (x 2)	188,900
PO Surge Tank	159,300
MW Collector	366,400
PG Collector	159,300
Total Bare Module Cost	$1,917,200

Total Capital Investment

C_{TBM} = $1,917,200

Ignoring costs of site preparation and service facilities, the direct permanent investment is:

C_{DPI} = $1,917,200

and the cost of contingencies and contractor fees is:

$C_{\text{cont}} = 0.18\, C_{\text{DPI}}$ = $345,000

Adding, the total depreciable capital is:

C_{TDC} = $2,262,300

Ignoring costs of land, royalties and plant startup, the total permanent investment is:

C_{TPI} = $2,262,300

Working capital, C_{WC}:

Number of batches in 30 days = 210
Price of propylene glycol = $*X*/lb
Accounts receivable = (210 batches)(2,636 lb/batch)($*X*/lb) = $553,600*X*

Number of batches in 2 days = 14
Price of propylene oxide = $0.72/lb
Total amount of PO needed = 2,500 lb/batch
2 day raw material inventory = (14 batches)(2,500 lb/batch)($0.72/lb) = $25,200

C_{WC} = \$25,200 + \$553,600X

Adding the working capital to the total permanent investment, gives the total capital investment:

C_{TCI} = \$2,287,500 + \$553,600X

Total Annual Production Cost

C = (\$1,238 + \$1,800) * 2,306 = \$7,006,000

Price of propylene glycol = \$$X$/lb
Total mass of PG produced = 2,636 lb/batch
Total sales = \$2,636X/batch
Total annual sales:

S = \$2,636X * 2,306 = \$6,079,000X

Propylene Glycol Selling Price

Rate of return on investment = 0.2 $= \dfrac{(1-t)(S-C)}{C_{\mathrm{TCI}}} = \dfrac{(1-0.37)(6{,}079{,}000X - 7{,}006{,}000)}{2{,}287{,}500 + 553{,}600X}$

Solving for X, X = \$1.31/lb

To achieve a rate of return on investment of 20%, the selling price of propylene glycol must be at least \$1.31/lb. This price is higher than that for the base case design (\$1.25/lb). Although the number of batches is higher in parallel operation, this mode of operation is less efficient for two reasons. First, the utility costs are higher for each batch, because the two columns are brought to total reflux before distillate is collected. In addition, the equipment costs are higher, because two smaller units are used in place of one; that is, the cost per unit volume is reduced due to smaller economies of scale.