

## Nomenclature

AR: Annual revenue  
B<sub>1</sub>, B<sub>2</sub>: Constants  
C<sub>1</sub>, C<sub>2</sub>, C<sub>3</sub>: Constants  
C<sub>BM</sub>: Bare module equipment cost  
cw: Cooling water  
CEPCI: Chemical Engineering Plant Cost Index  
C<sub>GE</sub>: Cost of general expense  
C<sub>GR</sub>: Grassroots cost  
C<sub>OL</sub>: Cost of operating labor  
C<sub>p</sub><sup>o</sup>: Purchase cost for base condition  
COM: Cost of manufacturing (without depreciation)  
COM<sub>d</sub>: Cost of manufacturing (with depreciation)  
C<sub>RM</sub>: Cost of raw materials  
CS: Carbon steel  
C<sub>TM</sub>: Total module cost  
C<sub>UT</sub>: Cost of utilities  
C<sub>WT</sub>: Cost of waste treatment  
D: Diameter  
DEG: Di-ethylene glycol  
EO: Ethylene oxide  
F<sub>BM</sub>: Bare module cost factor  
FCI: Fixed capital investment  
F<sub>M</sub>: Material of construction factor  
F<sub>p</sub>: Pressure factor  
F<sub>q</sub>: Tower factor  
hps: High pressure steam  
K<sub>1</sub>, K<sub>2</sub>, K<sub>3</sub>: Constants  
L: Length  
MEG: Mono-ethylene glycol  
N: Numbers of tray  
N<sub>OL</sub>: number of operators per shift  
N<sub>NP</sub>: number of processing operations  
P: Pressure  
SS: Stainless steel  
SF: stream factor  
ROI: Return on investment  
V: volume

## Executive Summary

The production of mono-ethylene glycol (MEG) is extensively studied in chemical industry as it lends itself to a wide array of applications. For this reason, it is necessary to optimize the design of such chemical plant and assess its viability. The purpose for this project was to simulate a catalytic thermal hydration of ethylene oxide (EO) to produce mono-ethylene glycol. The challenge faced in simulating this process was obtaining a 5000 kg/hr production rate of MEO with a 99 wt% purity while maintaining a 90% selectivity toward MEG and a H<sub>2</sub>O/EO ratio of 22. This was addressed by prepping (1) the feed stream (H<sub>2</sub>O and EO) to the reactor favorable operating conditions, (2) separating the desired (MEG) product from its byproduct (DEG) using a two-stage distillation system, (3) recycling water to the reactor during the separation, and (4) bringing the product stream to atmospheric conditions. The project was simplified in that the only side-product oligomer considered in the reaction was di-ethylene glycol. The next step in the project would be to simulate a nearly pure and selective MEG production plant while accounting for other oligomer byproducts.

# Table of Contents

<b>Nomenclature .....</b>	<b>ii</b>
<b>Executive Summary .....</b>	<b>iii</b>
<b>List of Figures .....</b>	<b>v</b>
<b>List of Tables .....</b>	<b>v</b>
<b>Introduction .....</b>	<b>1</b>
<b>Process representation .....</b>	<b>2</b>
<b>Process set-up .....</b>	<b>7</b>
<b>Feed preparation .....</b>	<b>7</b>
<b>Reactor .....</b>	<b>7</b>
<b>Separation .....</b>	<b>8</b>
<b>Recycle .....</b>	<b>9</b>
<b>Case studies .....</b>	<b>9</b>
<b>Cost analysis.....</b>	<b>13</b>
<b>Capital cost.....</b>	<b>13</b>
<b>Operating Costs .....</b>	<b>14</b>
<b>Conclusion.....</b>	<b>15</b>
<b>References .....</b>	<b>16</b>
<b>Appendix A: Sample Calculations.....</b>	<b>17</b>
<b>Appendix B: Supplemental tables and figures .....</b>	<b>23</b>
<b>Appendix C: Task allocation .....</b>	<b>27</b>
<b>Appendix D: Personal ethics agreement.....</b>	<b>28</b>

## List of Figures

Figure 1: Process block flow diagram (BFD) .....	3
Figure 2: Process flow diagram (PFD).....	3
Figure 3: Piping and instrumentation diagram (P&ID) .....	4
Figure 4: Effect on changing molar ratio of feed streams on condenser duty for column 1 .....	10
Figure 5: Effect on changing molar ratio of feed streams on condenser duty for column 2 .....	10
Figure 6: Effect of changing molar ratio of feed streams on MEG product flow .....	11
Figure 7: Effect on changing molar ratio of feed streams on reboiler duty for column 1 .....	11
Figure 8: Effect on changing molar ratio of feed streams on reboiler duty for column 2 .....	12
Figure 9: Effect of changing molar ratio of feed streams on MEG product purity.....	12

## List of Tables

Table 1: Process specifications for UNISIM simulation .....	1
Table 2: Flow summary table.....	5
Table 3: Equipment summary table.....	6
Table 4: Pumps used for feed preparation .....	7
Table 5: Summary of pump and heat exchanger characteristics for processing of recycle stream	9
Table 6: Operating cost summary breakdown .....	14
Table 7: Fixed capital investment .....	14
Table 8: Cost of utilities and materials .....	14
Table 9: Cost of manufacturing.....	15

## Process set-up

### Feed preparation

The two feed streams had to be modified to get to the conditions necessary for the reactor. It was decided to pump the streams first and then heat them before mixing them and sending the mixed stream to the reactor. The reason for pumping the streams first was that if the temperature was raised first then vapour would be present. With vapour present it would be necessary to use expanders which are usually more expensive than pumps [8]. The operating conditions for the pumps can be seen below in table

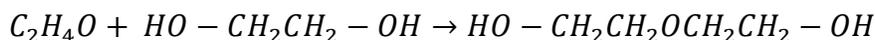
Table 4: Pumps used for feed preparation

Pumps	P-101	P-102
Flow (kg/h)	36070	4009
Fluid density (kg/m <sup>3</sup> )	1007	885.2
Power (kW)	18.81	2.046
Type		
Efficiency	75%	75%

To bring the streams to the temperature needed for the reactor a heat exchanger with high pressure steam was used. The steam is at a temperature of 280°C and the condenses to provide the heat. The flow rates of steam were 12020 and 1866 kg/h of steam for E-101 and E-102 respectively.

### Reactor

The reactor conditions were provided as seen in table 1. The temperature was 150°C and the pressure was 1.5Mbar. There were two reactions which occurred, the main reaction as well as one side reaction.



## Operating Costs

Operating cost for the process were summarized as follow:

**Table 6: Operating cost summary breakdown**

Operating labour cost	900000	
MEG production (tonne / h)	5.003	
3 operators per shift	15	operators
Operator salary (\$/year)	60000	
Working hours per year (h/y)	8736	
Cost of labour (\$/h)	900000	

The fixed capital investment was obtained from the Grass root cost (March 2017)

**Table 7: Fixed capital investment**

FCI	1288655
-----	---------

Water was recycled in this process and there was not any waste water treatment. Next, the cost of utilities along with material costs were calculated and the result were summarized as follow:

**Table 8: Cost of utilities and materials**

Cost of utilities	5.3E+07	Cost of raw materials	5.6E+07
Total cooling water mass fowrate (kg/h)	32410.9	H <sub>2</sub> O mass flowrate (kg/h)	36066.2
Total high pressure steam mass fowrate (kg/h)	1.66E+06	EO mass flowrate (kg/h)	4008.91
Cooling water price (\$)	14.8	H <sub>2</sub> O price	-
High pressure steam price (\$)	29.97	EO price (\$/kg)	1.687
Total cooling water cost (\$)	4E+07	H <sub>2</sub> O raw material cost	-
Total high pressure steam cost	1.4E+07	EO raw material cost	5.6E+07
Total utility cost (\$)	5.3E+07		

From there, the cost of manufacturing was calculated. The cost of manufacturing (March 2017) was found to be \$132, 285 681.6 with a revue of \$ 673 051 70.83 and an annual profit of \$ 69, 688 186.26: