

Numerical Modelling and Simulation Recovery Unit of Monoethylene Glycol from Affluent Debris of Indorama Eleme Petrochemical Limited Nigeria

Engr. Nnadikwe Johnson

*Department of Chemical Engineering
Imo state Polytechnic, Owerri Nigeria*

Engr. Unyime Enobong Okure

*Department of Chemical Engineering
Imo state Polytechnic, Owerri Nigeria*

ENGR. IHEME CHIGOZIE

*Department of Chemical Engineering
Imo state Polytechnic, Owerri Nigeria*

Engr. Benedict Okon Edensetang

*University of Uyo, Uyo
Nigeria*

ABSTRACT

Rising oil prices and environmental concerns have prompted chemical and petrochemical businesses to recycle more waste. This research studied Indorama Eleme Petrochemical Limited's glycol separation and recycling. The petrochemical company didn't contemplate a waste recovery facility, and it looks a new unit is needed. Using Aspen Hysis modeling software, glycols were extracted from water/salt mixtures. Simulator sensitivity was analyzed to enhance the approach. MEG, DEG, TEG, and TTEG may be recycled at 5.01, 2.039, 0.062, and 0.089 flow rates.

Keywords: Glycol, Aspen, Water, Salt, Distillation

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I. INTRODUCTION

Polyhydroxy compounds like glycols and glycerol are hard and costly to recover from water. PG and EG are industrial compounds created by hydrating epoxides in water. Pure PG and EG must be extracted from aqueous solution, which requires a lot of energy. Vacuum distillation reduces energy expenditures and temperatures, eliminating polyglycols and breakdown products.

Feng et al. [1] pervaporated chitosan membranes to extract water from ethylene glycol. According to the results, conditioning the pervaporation membrane at maximum operating temperature altered membrane permselectivity. Huang et al. [2] studied pervaporation separation of ethylene glycol aqueous solutions. In separation operations, heat relieved membrane relaxation. Before steady-state transport is achieved, the feed mix swelling relaxes the heat-treated pervaporation membranes. Examining membrane sorption and pervaporation separation.

Dhale et al. [3] employ cationic exchange resins as catalysts in bench- and pilot-scale continuous RD columns to extract PG and EG from water. Hydrolysis of acetals to remove glycols uses the same columns. Based on bench-scale experiments, a pilot-scale device was built. PG acetalization was simulated using the RADFRAC module of Aspen Plus 11.1. According to simulations of commercial-scale acetal synthesis from PG, a 25-step RD column can recover all PG from aqueous solution. Mohammadi and Akbarabadi [4] established the possibility of employing VMD to concentrate ethylene glycol (EG). VMD studies were conducted using water-

EG combinations using a flat-sheet polypropylene membrane at different temperatures and recirculation rates. The membrane rejects EG nearly completely, and the proper concentration was reached.

Guo et al. [5] dehydrated ethylene glycol (EG) aqueous solution by pervaporation via a crosslinked poly(vinyl alcohol) membrane. Good thermal, mechanical, and pervaporation properties (at 70°C for an EG aqueous solution containing 80% EG).

KHARG MEG is one of Iran's biggest glycol facilities, with 7920 production hours per year. Salt, water, and glycols from plants aren't recycled and instead dumped in the environment. In this investigation, we'll aim to recover glycols from plant waste. We'll use Aspen Simulation Software.

II. METHODOLOGY

Plant has three waste streams. NaHCO₃ and glycols and water are process inputs. Simulated plant waste combination was 764 kg/h. These streams are:

Table 1. The definition of feed streams

| Name | Feed 1 | Feed 2 | Feed 3 |
|---------------------------|-------------|------------|--------------|
| Temperature (C) | 120/4 | 166/9 | 186/1 |
| Pressure (bar) | 1/42 | 1/420 | 1/420 |
| Vapor Frac | 0 | 0 | 0 |
| Mole Flow (kmol/hr) | 13 | 4 | 0/18 |
| Mass Flow (kg/hr) | 416 | 317 | 31 |
| MEG (kg/h) | 212/2 | 99/9 | 0 |
| DEG (kg/h) | 0 | 208/7 | 0 |
| TEG (kg/h) | 0 | 0 | 13/1 |
| TTEG (kg/h) | 0 | 0 | 18/1 |
| H ₂ O (kg/h) | 166/6 | 0/1 | 0 |
| NaHCO ₃ (kg/h) | 37/7 | 8/4 | 0 |

Aspen Plus Simulator 8.6 was utilized. Activity coefficients were calculated using the NRTL thermodynamic model for electrolytes [6-7]. Figure 1 shows the simulation's flowchart.

A salt/water/glycols solution is supplied to a first separation column at an intermediate step. In the separation column, water and glycols are the top and bottom products, respectively. This mixture is heated to 119°C in a heat exchanger before being fed to a water-glycol separation column. Bottom glycols were transported to glycol separation columns. Separate MEG, DEG, TEG, and TTEG.

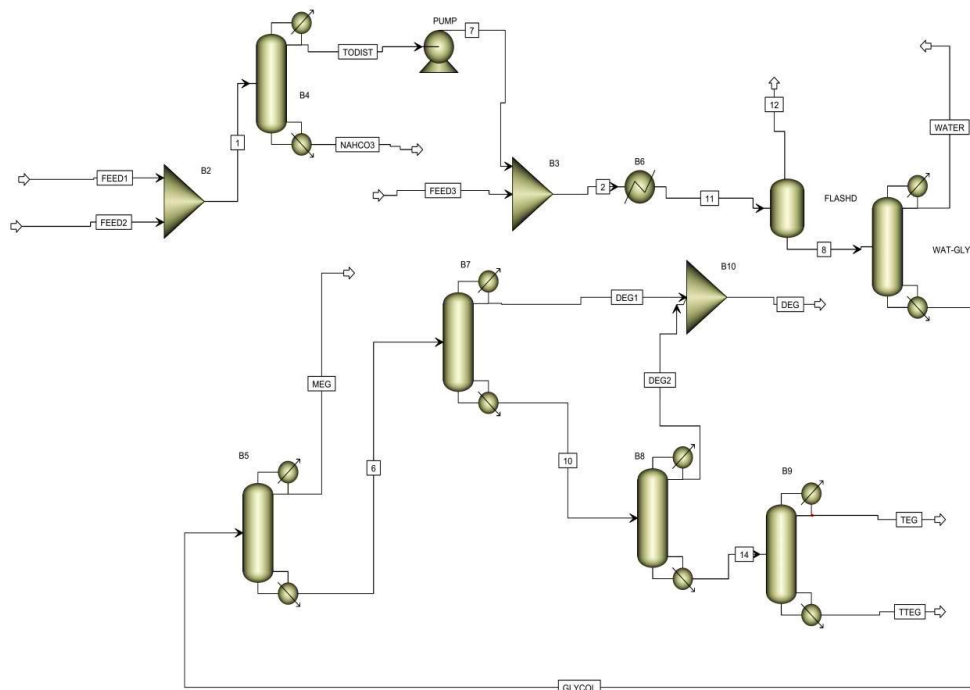


Figure 1. Diagram of the process

III. Thermodynamic Model

a. SIMULATION OF A PROCESS

First, Aspen Tech's vapor-liquid pseudo-binary equilibrium simulation in the Aspen Split confirmed the thermodynamic model.

The following equations are used to model a binary mixture:

$$\begin{cases} \ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1+x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2+x_1 G_{12})^2} \right] \\ \ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2+x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1+x_2 G_{21})^2} \right] \end{cases} \quad (1)$$

With:

$$\begin{cases} \ln G_{12} = -\alpha_{12} \tau_{12} \\ \ln G_{21} = -\alpha_{21} \tau_{21} \end{cases} \quad \alpha_{12} \quad (2)$$

Inhere τ_{12} and τ_{21} may be used to describe the non-dimensional interactions between two objects and by:

$$\begin{cases} \tau_{12} = \frac{\Delta g_{12}}{RT} = \frac{U_{12}-U_{22}}{RT} \\ \tau_{21} = \frac{\Delta g_{21}}{RT} = \frac{U_{21}-U_{11}}{RT} \end{cases} \quad (3)$$

U_{ij} , or the energy between molecular surfaces j and i is given by R and T , respectively. Evaporation energy is referred to as U_{ii} . In this case, U_{ij} and U_{ji} must be equal but Δg_{ij} is not necessary equal to Δg_{ji} . The parameters α_{12} and α_{21} are the so-called non-randomness parameter, for which usually α_{12} is set equal to α_{21} . For a liquid, in which the local distribution is random around the center molecule, the parameter. In that case the equations reduce to the one-parameter Margules activity model:

$$\begin{cases} \ln \gamma_1 = x_2^2 [\tau_{21} + \tau_{12}] = A x_2^2 \\ \ln \gamma_2 = x_1^2 [\tau_{12} + \tau_{21}] = A x_1^2 \end{cases} \quad (4)$$

Most of the time, it's between 0.20 and 0.48. For aqueous systems, this value is often utilized. Hydrogen bonding are responsible for the structure's high value. The non-randomness value is set to 0.2 in the explanation of liquid-liquid equilibria, however. It is possible in certain circumstances to describe equilibria more accurately by establishing parameters $\alpha_{12} = -1$. Physically, no system can be more random than random, hence this mathematical solution is unattainable ($\alpha_{12}=0$). NRTL's additional non-randomness characteristics provide for greater flexibility in describing phase equilibria than other activity models. In reality, this flexibility is restricted to prevent erroneous equilibrium descriptions outside of regressed data [8-10].

a) Configuration

This research examined the reflux ratio, separation stages, and feed temperature. Table 2 lists column parameters. When creating the model, sensitivity studies and plots were utilized to show the influence of variables on a design condition. Each column's reboiler energy usage and distillate composition, which should be 99 percent glycols, were analyzed. The first column's bottom pressure should be less than 0.01bar to minimize heat problems.

Table 2. Column parameters

| | B4 | WATER-GLYCOL | B5 | B7 | B8 | B9 |
|-------------------------|--------------|--------------|--------------|--------------|--------------|--------------|
| Calculation type | Equilibrium | Equilibrium | Equilibrium | Equilibrium | Equilibrium | Equilibrium |
| Number of stage | 10 | 17 | 20 | 20 | 20 | 20 |
| Condenser | Total | Total | Total | Total | Total | Total |
| Reboiler | Kettele | Kettele | Kettele | Kettele | Kettele | Kettele |
| Valid phases | Vaper-Liquid | Vaper-Liquid | Vaper-Liquid | Vaper-Liquid | Vaper-Liquid | Vaper-Liquid |
| Convergence | Standard | Standard | Standard | Standard | Standard | Standard |
| Reflux ratio(Mass) | 0/1 | 0/6 | 5/01 | 1/95 | 0.89 | 0.62 |
| Bottoms ratio(kmole/hr) | 0/55 | 7/2 | 1/5 | 5 | 5 | 3 |
| | | | | | | |

IV. RESULTS AND DISCUSSION

4-1 Glycol column

Figure 2 shows the water-glycol separation column's pressure-temperature curve. Rising column pressure increases reboiler duty, as shown. Figure 3 shows reboiler and condenser duty at different pressures. Rising pressure increases boiler duty while lowering condenser duty, graph shows. Increased pressure makes liquid condensing simpler, reducing condenser load.

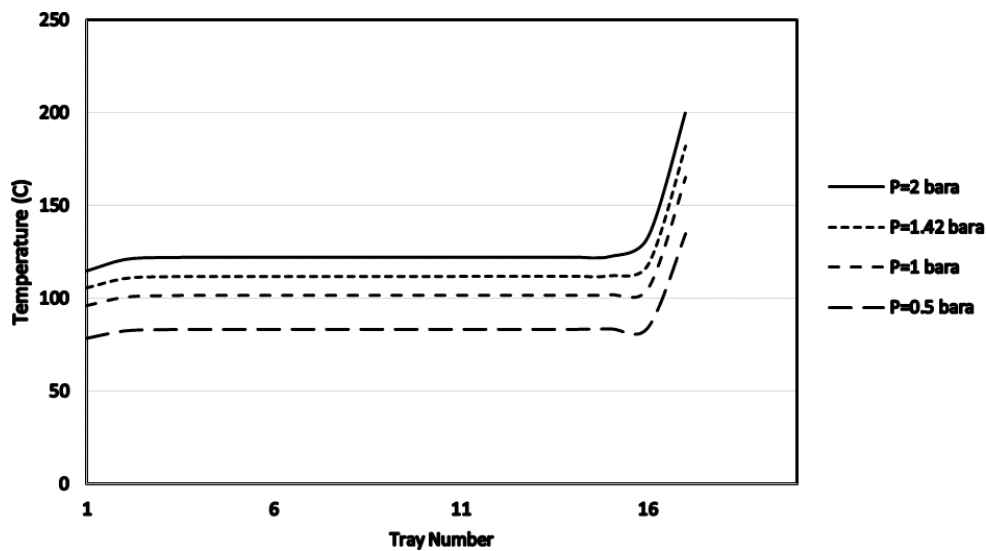


Figure 2. Water-glycol column temperature profile

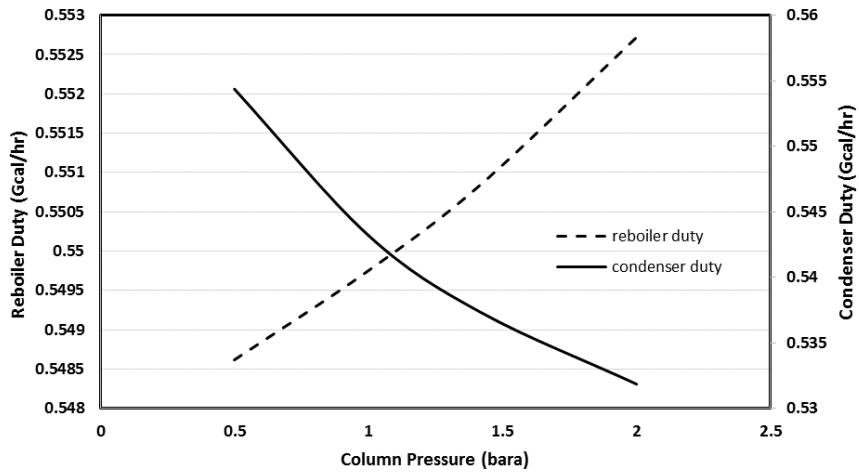


Figure 3. Water-glycol separation column reboiler and condenser

Reflux ratio is another important column performance factor. Figure 4 shows that increasing the reflux ratio increases reboiler and condenser duty. Because the overhead product is water, increasing the reflux ratio is not suggested.

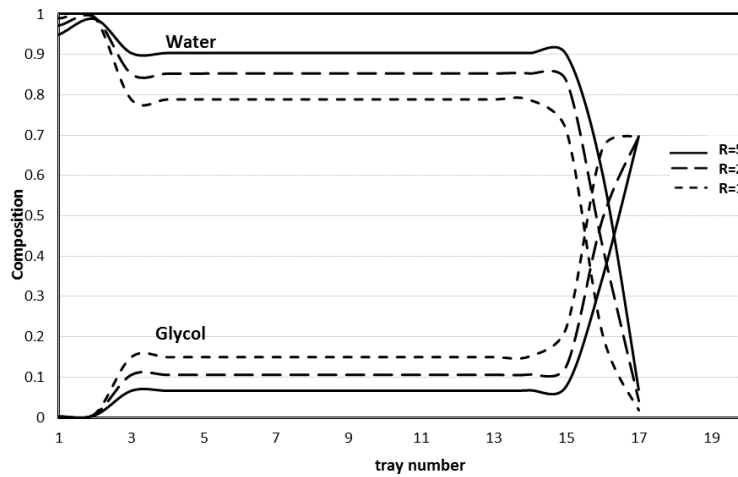


Figure 4. Water-glycol separation column tray-by-tray product profile variation

4-2- MEG separation:

Figure 5 shows the MEG temperature curve. Similar to the water-glycol separation column, increasing pressure boosts column temperature, increasing reboiler duty and decreasing condenser duty (figure 6).

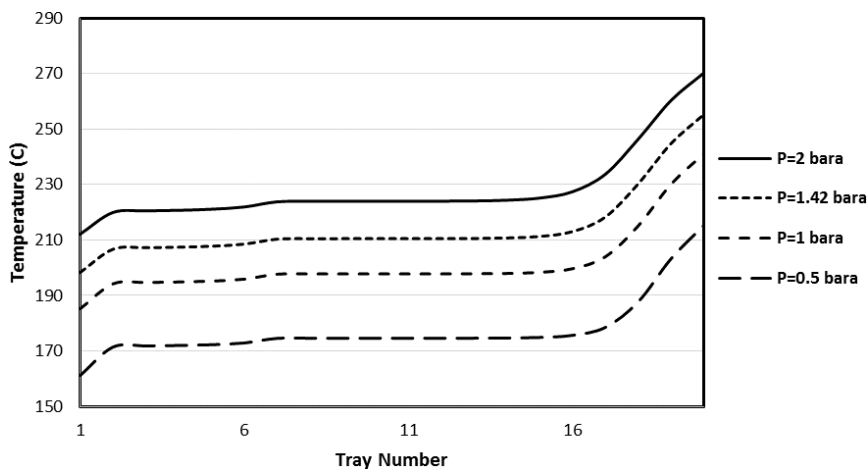


Figure 5. MEG column temperature profile

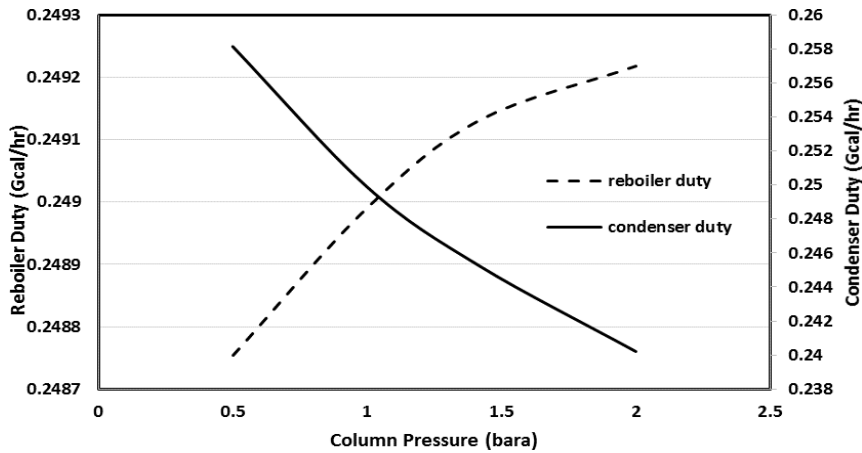


Figure 6. MEG column reboiler and condenser

Figure 7 indicates that raising reflux ratio increases product purity. Reboiler and condenser duty increase energy and operating costs. MEG column separation optimum was 1.5.

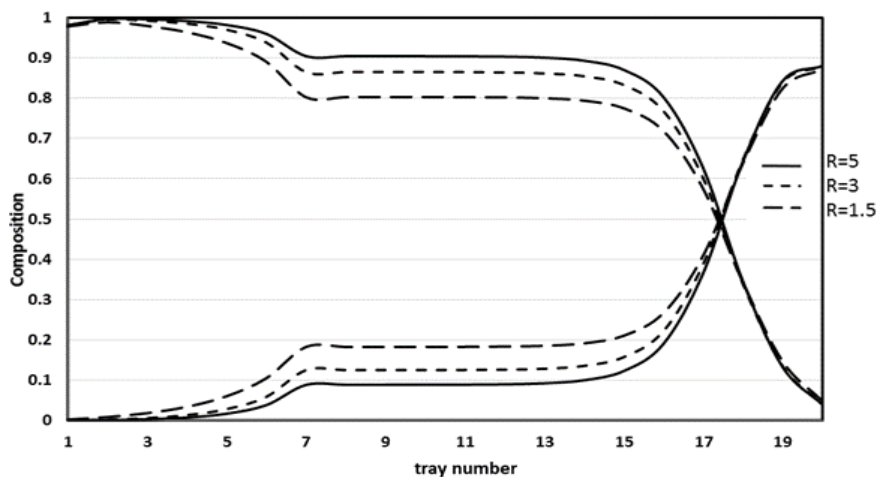
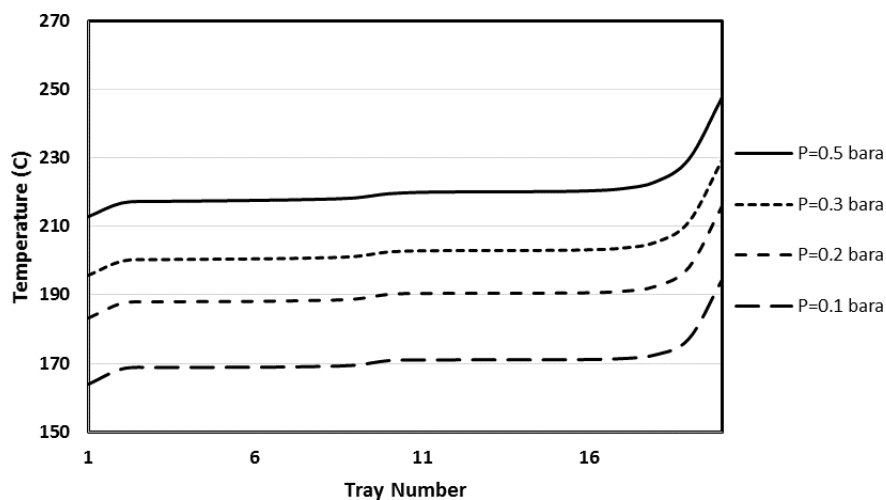


Figure 7. MEG separation column tray-by-tray product profile variations

4-3- DEG separation columns:

Because DEG couldn't be entirely separated from glycols, a distillation column was recommended. Figure 8 shows column temperatures at different pressures. Increased pressure results in greater temperatures at each tray, as seen in the figure. As pressure increases, reboiler duty drops. Figure 9 shows 1 bara column pressure. High temperature destroys glycols and lowers process efficiency, even if increased pressure reduces reboiler duty. Lowering column pressure is sensible.



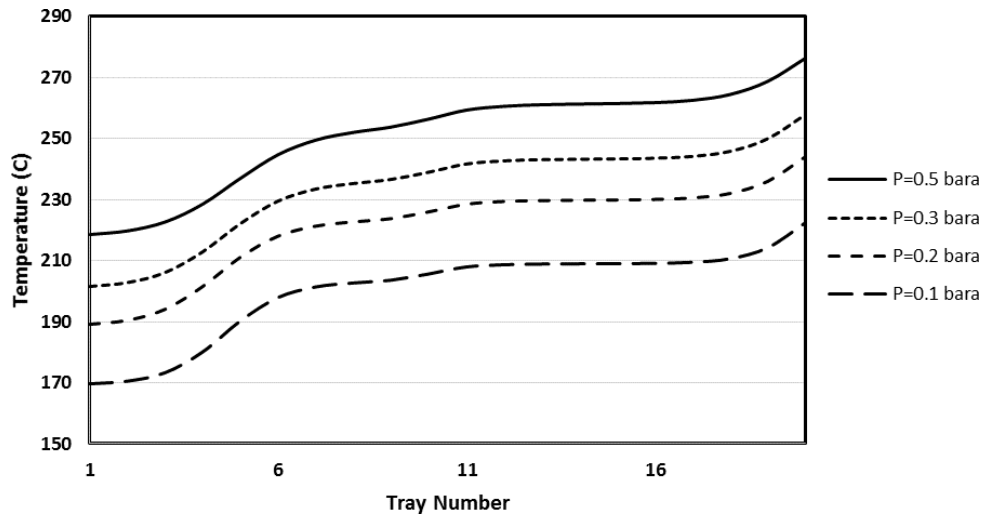


Figure 8. DEG-1 and DEG-2 column temperatures

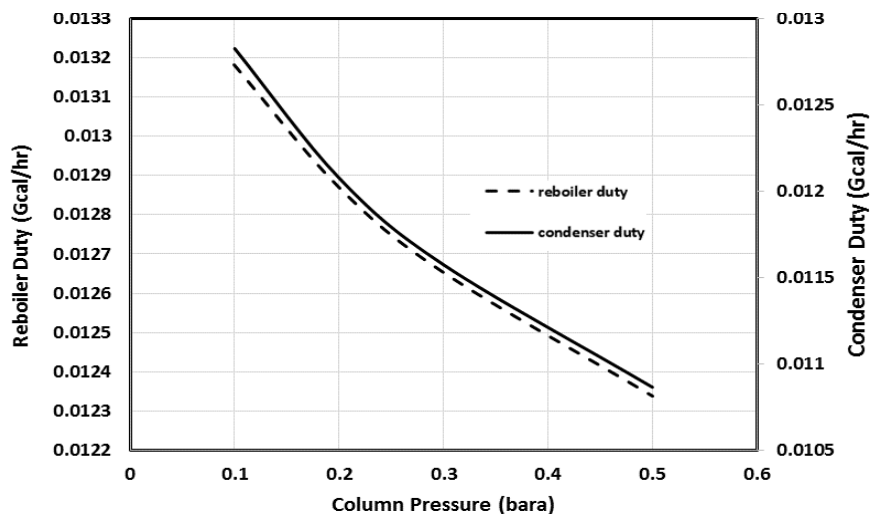
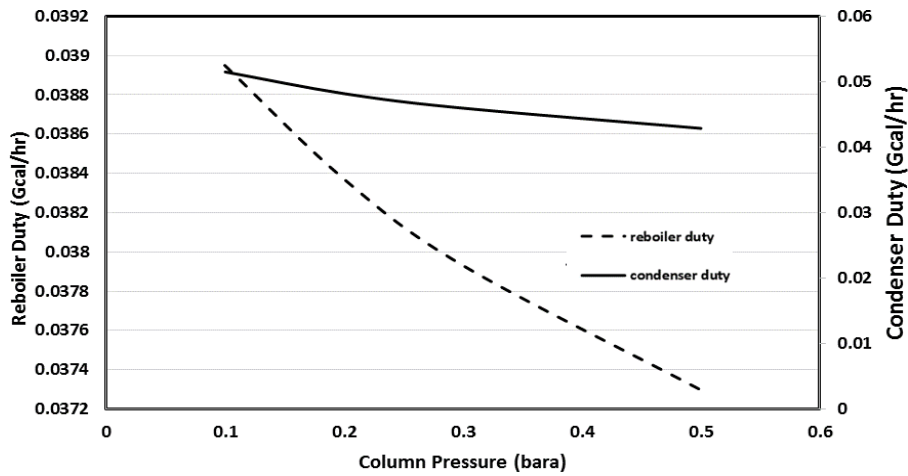


Figure 9. Reboiler/condenser for DEG-1 and DEG-2 columns

Comparing boilup ratios indicates none affect product quality. This column's boilup ratio is 5.

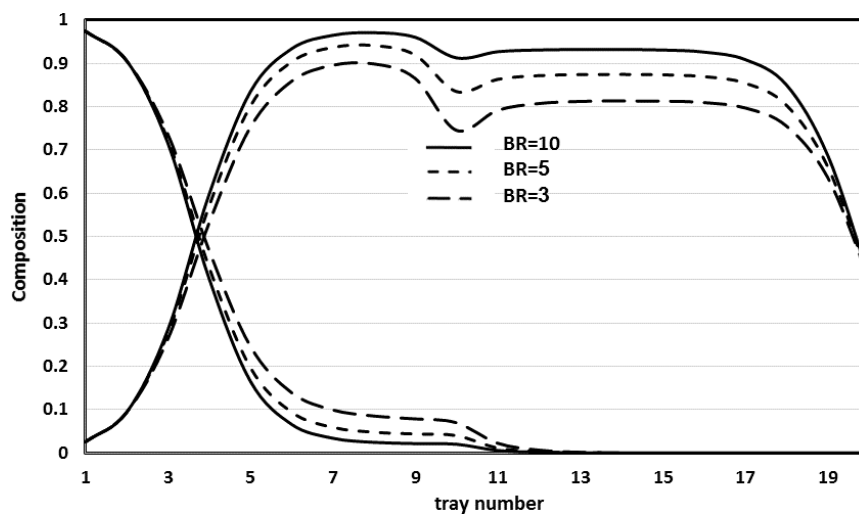
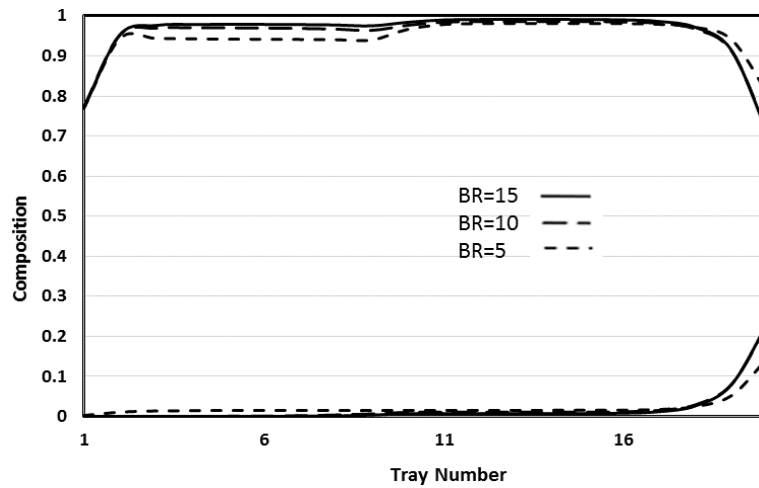


Figure 10. Water-glycol separation column tray boilup ratio affects product profile.

4-4- TEG and TTEG column:

Last column's top product is TEG and bottom is TTEG. Figure 11 displays this column's temperature profile. As seen, increasing pressure boosts tray temperatures and reboiler duty (Figure 12). Increasing temperature degrades glycols, which isn't good for column alteration.

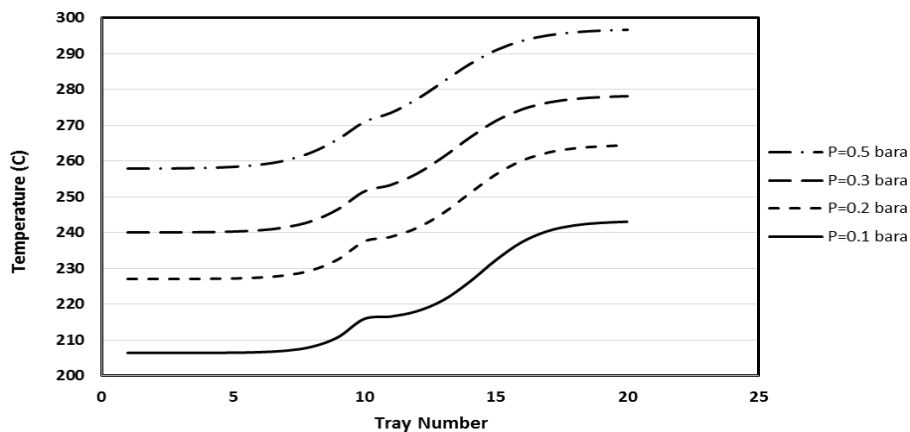


Figure 11. TEG-TTEG column temperature profile

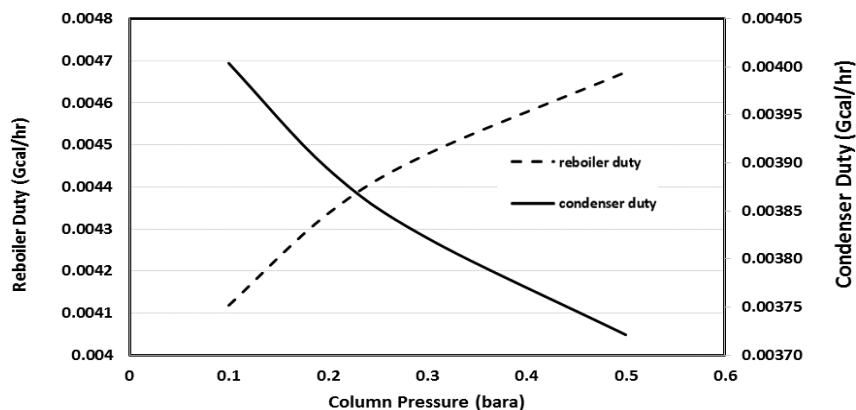


Figure 12. TEG-TTEG separation column reboiler and condenser

Figure 13 shows how reflux ratio affects column performance. Raising the reflux ratio increases product purity and thermal duty, as shown. This column's reflux ratio is 3.

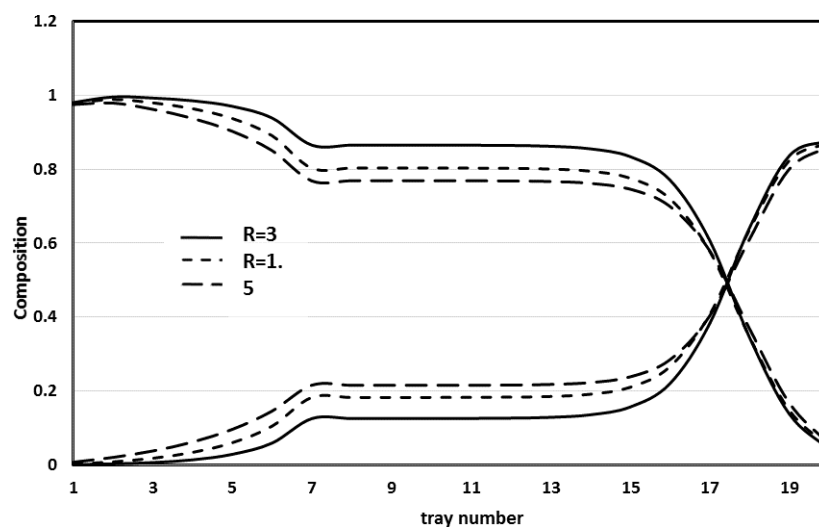


Figure 13. TEG-TTEG separation column tray-by-tray product profile variant

After adjusting all columns' performance, MEG, DEG, TEG, TTEG may be recycled with a flow rate of 5.01, 2.039, 0.062, and 0.089.

V. CONCLUSION

This research examines a procedure for separating water, salt, and glycols. Aspen Plus simulated the procedure. After adjusting all columns, MEG, DEG, TEG, and TTEG may be recycled at flow rates of 5.01, 2.039, 0.062, and 0.089.

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