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Research Article

Production of Monoethylene Glycol via Reactive Distillation Column

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Abstract: Monoethylene Glycol is a widely used chemical and is a crucial component in the manufacturing of polyester film and fibers, Polyethylene Terephthalate (PET) resins and engine coolants. Monoethylene glycol application ranging from clothing and textiles, kitchenware, engine coolants, antifreeze, and packaging. In 2011, the global usage and production of monoethylene glycol reach 20 million metric tons and is expected to increase 5-10% each year. However, conventionally the production of Monoethylene Glycol is not considered as a sustainable process since it is known as an energy intensive process. Production of Monoethylene Glycol usually involves excess water and the ratio of water to ethylene oxide is 20:1. Besides that the conversion of this process also did not reach maximum conversion. By applying reactive distillation column to replace the conventional process the problems stated above can be solved. Analysis for the selectivity, conversion, process mass intensity, heat and pressure will result in higher selectivity toward product, maximum conversion, lesser capital investment and lower energy usage. The simulation and modelling for this process will be carried out in ASPEN Plus™. The result from this simulation is by using lesser molar ratio of water and ethylene oxide the conversion is bigger than 99% and the process mass intensity of reactive distillation column is 1, where all the raw material is converted to monoethylene glycol.

Keywords: Monoethylene glycol, Reactive Distillation Column, ASPEN Plus

1. Introduction

Monoethylene Glycol is the simplest organic compound in the glycol group. The glycol group is an alcohol that has two hydroxyls besides a carbon atom. It is an odorless, clear, sweet-tasting, and viscous compound that has the boiling point of 198°C. Table 1 shows the Monoethylene Glycol introduction summary and Table 2 shows the physical properties of monoethylene glycol.

Table 1. Monoethylene Glycol introduction summary

<i>Name:</i>	<i>Monoethylene Glycol</i>
IUPAC Name:	1,2-ethanediol
Other Name:	Ethylene Glycol
CAS Registry:	107-21-1
Chemical Structure:	HOCH ₂ CH ₂ OH

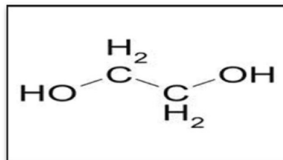


Figure 1. Chemical structure of Monoethylene Glycol

Table 2. Physical properties of Monoethylene Glycol

<i>Properties</i>	<i>Value</i>
Boiling Point	198 °C
Freezing Point	-11.2 °C
Molecular Weight	62.07 g mol ⁻¹
Solubility in water at 20°C	100 wt%
Water Solubility in Monoethylene Glycol at 20°C	100 wt%
Critical Pressure	8,200 kPa
Critical Specific Volume	0.191 L g ⁻¹ mol ⁻¹
Critical Temperature	446.85 °C
Density	1.11 g cm ⁻³
Higher homologues	Diethylene Glycol Triethylene Glycol Polyethylene Glycol

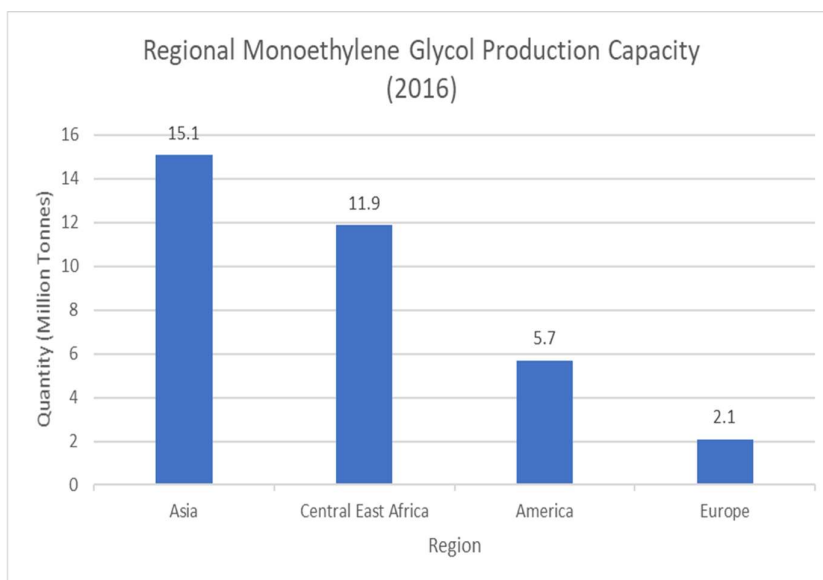


Figure 2. Regional Monoethylene Glycol Production Capacity (2016)

Asia gives the largest monoethylene glycol production capacity in 2016. This occurs due to Asia fiber and textile production where both of this production demand a large amount of monoethylene glycol thus leads to 15.1 million tonnes of Monoethylene glycol production.

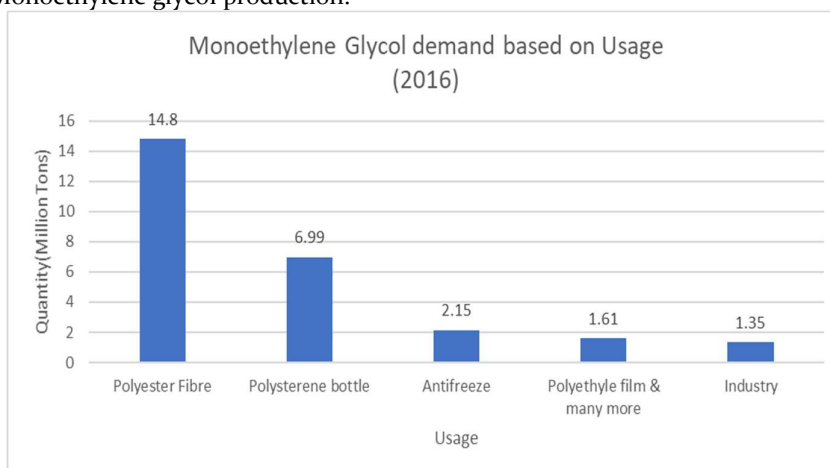


Figure 3. Monoethylene Glycol demand based on Usage(2016)

Monoethylene glycol demand depend on its usage. In Figure 3, the demand from the polyester fiber reach 14.8 million tons per year while from polystyrene bottle production reach 6.99 million tons per year. Meanwhile the demand for antifreeze, polyethylene film and industry are 2.15, 1.61, 1.35 million tonnes per year. Monoethylene glycol is an important raw material in industrial usage. Monoethylene glycol is used as engine coolant, antifreeze material and the main raw material for polyester fiber, resins and in cosmetic applications (H. Yue et. al. 2012).

1.2 Hydration of Ethylene Oxide

In the hydration process of ethylene oxide to form monoethylene glycol. The reaction will conventionally produce the higher homologue of Monoethylene glycol which is diethylene glycol and triethylene glycol.



Equation 1 shows the intermediate ethylene, which is ethylene oxide, C_2H_4O will reacts with water which will produce ethylene oxide. This reaction can be catalyst by acid, bases, and normal pH with high temperature. Other product also can be formed from this reaction like the oligomer of monoethylene glycol which is diethylene glycol and triethylene glycol. (Akpa et. al. 2018)

1.3 Conventional Process

Conventional process operates with huge abundance of water to ethylene oxide on a molar ratio of 20:1. The abundance of water is used to reduce the production of the higher homologues of ethylene glycol. Ethylene oxide mixture which is heated to 200°C is fed to continuous stirred tank reactor with water. The reactor will operate at 190°C-200°C and at a pressure of 14-22 atm. The selectivity of the reaction between ethylene oxide and ethylene glycol is higher than the selectivity of the main reaction hence the water is added in abundance to reduce diethylene glycol from the process. The mixture of water will then enter a multiple stages dehydrator to separate the water from ethylene glycol. Then the monoethylene glycol will go through multiple distillation columns to separate the monoethylene glycol and it higher homologues. (Melhem et. al. 2001) Figure 4 illustrates the conventional process to produce monoethylene glycol.

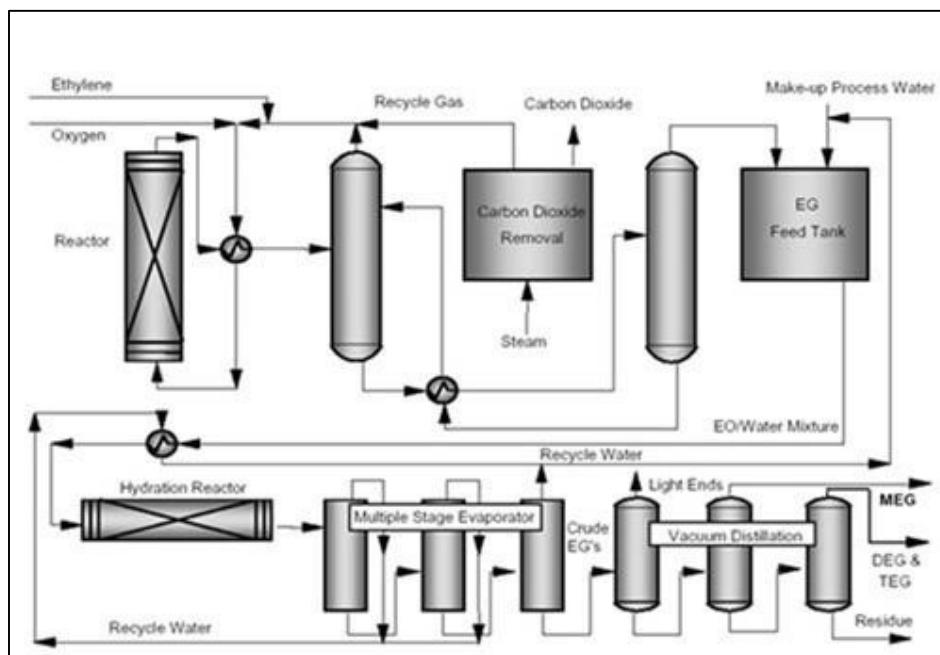


Figure 4. Conventional process for MEG production

There are a few issues regarding using conventional process to produce monoethylene glycol. Conventional process using a separate reactors and distillation column have a low conversion rate without the massive abundance of water to ethylene oxide ratio which is 20:1. (Lianghui Ding 2019) Conventional process is said to be energy-intensive because of the large amount water released from this process and the high consumption of energy, (Akpa et. al. 2018)

The disadvantages of conventional process can be overcome by using reactive distillation column. Reactive distillation is a process where separation and reaction happen in a column that has many advantages especially in optimal condition. Besides, this process combine the benefit of chemical equilibrium and distillation to reach higher improvement in promoting higher conversion in reaction. (Saidat Olanipekun et. al. 2017)

Although distillation is the oldest separation process and is the most commonly used in industry, there is many ways to improve the distillation process.(Anton A. Kiss 2013) In the various advances that have been developed as a method of intensification of the distillation process, the reactive distillation column which combines chemical reaction and separation is the most advanced method of process intensification because this method can increase conversion rate and selection, reduce energy consumption, and bring a process leading to process sustainability.(Anton A. Kiss 2019)

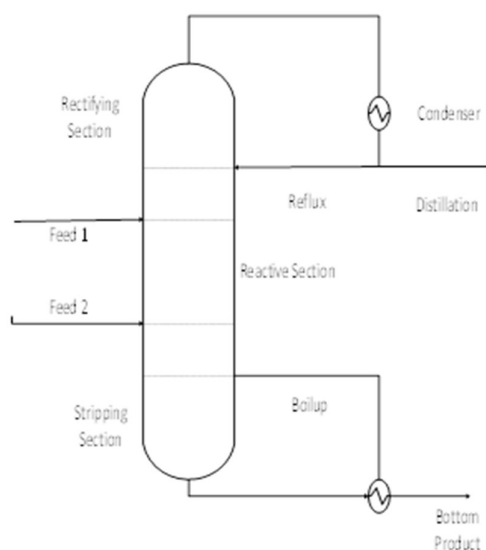


Figure 5. Reactive Distillation Column Process Structure

Figure 5 shows the process structure of a reactive distillation column. The difference between conventional distillation column and reactive distillation column is reactive distillation column usually has 2 or multiple feed and have reaction section in the column where the reaction will happen.

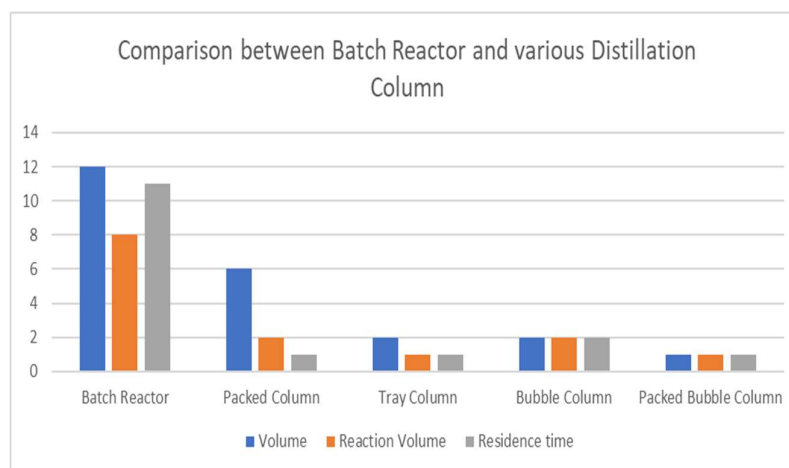


Figure 6. Comparison between reactor and various distillation column

The novel process reactive distillation column is used to synthesis polyester. This process is a new process that can reduce the production time with a better product quality with lower operational cost. The maximum conversion rate will be achieved within a shorter amount of time, and at the same time excessive water can be eliminated from the system. Reactive distillation system takes only 1.8-2 hours where the amount of time is significantly reduced compared to conventional process which will take 6-8 times longer. Figure 6 shows the volume, reaction volume and residence time of each the process. (Anton et. al. 2016)

1.4 Advantages and Disadvantages of Reactive Distillation Column

Table 3. Advantages and disadvantages of reactive distillation column

<i>Reactive Distillation Column Advantages</i>	<i>Reactive Distillation Column Disadvantages</i>
<i>Process Simplification</i>	Less Flexibility
<i>Capital saving</i>	
<i>Increased Conversion</i>	Operating window Constraint
<i>Increased Selectivity</i>	Reactive Azeotrope Occurrence
<i>Reduced Energy Saving</i>	
<i>Safety Intrinsic</i>	Occurrence of several steady state
<i>Overcome Azeotrope</i>	
<i>For low difference boiling component separation</i>	

Based on Table 3, there are many advantages and disadvantages that need to be considered before performing production through reactive distillation column. There are several advantages of reactive distillation column as this process helps in simplifying the process. Complex conventional process can be converted to reactive distillation columns which are easy to operate and inexpensive to operate as well as in terms of maintenance. Next, the reduction of capital investment, by reducing the utilities in operation, capital investment will also be reduced. In addition, the increase in conversion rate and selectivity is also an important advantage of reactive distillation columns. The conversion rate can be increased by this process because the removal of the product from the reaction part will cause the chemical balance of the reaction to change and will achieve a higher conversion rate, eventually the conversion rate will reach the maximum rate. Selection will also be product-oriented because the removal of the product from the reaction section will make the selection product-oriented. In addition, energy reduction can also be achieved by using this process. The exothermic heat from the reaction will aid the heating process and be able to reduce the duties of the boiler and condenser. Intrinsic safety is meant to be that naturally the reactive distillation column is a system where hot spots can be avoided, and hazardous chemicals can also be used in this reactive distillation column due to its relatively low liquid resistance. In addition, azeotrope can also be avoided by selecting certain conditions because azeotrope will be avoided during the reaction on the liquid phase. Lastly is the separation of liquids whose low boiling point differences can also be performed on reactive distillation columns. (Anton A. Kiss. 2019)

There are some constraints in performing a process that uses a reactive distillation column. First is the lack of process flexibility that occurs because the level of integration of this process is higher than that of processes that use conventional processes. In addition, this process also puts constraints on the operating window. Separation and reaction operations take place under the same conditions. So, a reasonable conversion rate with the conditions is required and considered for the distillation process. Reactive azeotrope will also occur using this process because the change in concentration that occurs due to distillation will affect the reaction. Reactive azeotrope will cause constraints on the distillation process and make the distillation process difficult or worst-case scenario the

distillation process cannot be implemented. Lastly is the occurrence of some steady state in the process. The complex interactions between chemical reactions and separations as well as other phenomena, make the behaviour of nonlinear processes more likely to occur with the possibility of some steady state. For this reason, the same reactive distillation head configuration operated under the same conditions can produce distillation head profiles with different steady states and will directly give different conversion rates. (Anton A. Kiss, 2019)

1.5 Catalyst

In a book by Shah et. al., the synthesis of unsaturated polyesters such as Monoethylene Glycol is a complex reaction and requires several types of reactions. There are several catalysts used to produce Monoethylene Glycol such as titanium, antimony and tin -based catalysts in various forms such as alkoxyene and even carboxylate. (de Haan AB et. al. 2013) Typically, catalysts in small amounts are used and practically left in Monoethylene Glycol, so separation and recovery of catalysts are avoided.

There are several types of reactions that can take place in a reactive distillation column. The first type is a non-catalytic reaction. This reaction will take place anywhere in the distillation column if reactants exist and for this process no catalyst is used, and no separation or recovery of the catalyst will take place. The second reaction is a reaction which uses a homogeneous catalyst. This reaction will also occur anywhere in the column. This catalyst will be left in one of the product streams or can be neutralized or separated by using a saltwater stream or separated from the product drain and recovered. Lastly, is the reaction using heterogeneous catalysts. There is a constraint on the reaction chamber because the catalyst used is a solid catalyst and this catalyst will not leave the reaction chamber and no recovery and separation process is required for this process. (Anton A. Kiss. et. Al. 2019)

2. Methodology

The software used for modeling this process is ASPEN Plus™. The interface example of ASPEN Plus™ is as shown in Figure 8. The thermodynamic feature package used is a non-random two-liquid model (NRTL) package because of the assumption that the reaction takes place in the liquid phase. The flow chart for this project is as shown in Figure 7. The project will begin by developing mathematical theories and models for reactive distillation columns.

There are a several analyses to be done in this process which are the comparison between selectivity, conversion, and yield between conventional and reactive distillation process. Next is the temperature, pressure, and composition analysis for reactive distillation column. Finally, is the effectiveness analysis between conventional process and reactive distillation column.

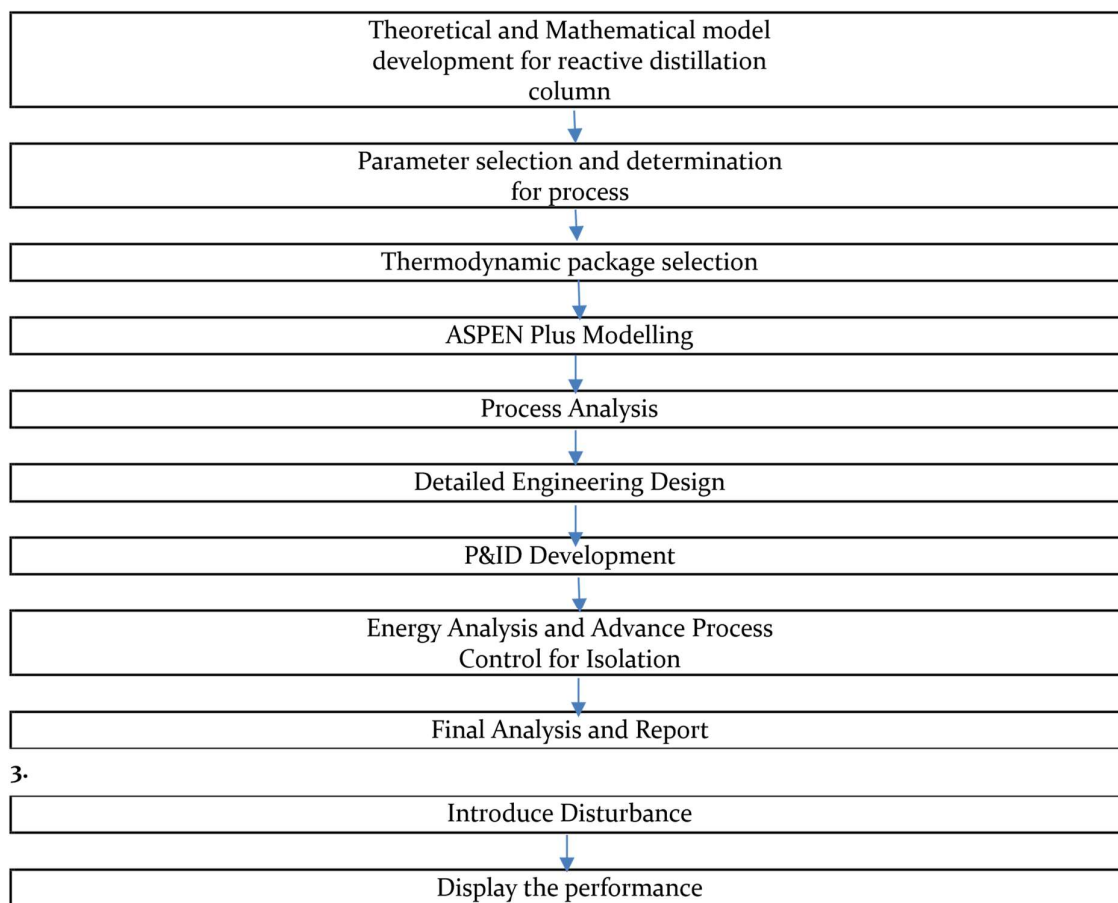


Figure 1. Procedure to evaluate the performance of control system.

4. Results and Discussion

The development of simulations and modeling of the production of Monoethylene Glycol has been carried out to obtain the values of selection, conversion and generally compare the effectiveness of the two processes. Process assumptions have been taken into account in running the simulation and modeling of this process. There were two processes compared and both of these processes were carried out as required modeling and simulation. The process is a process which uses a continuous stirring tank reactor (CSTR) and a process using a reactive distillation column. The flow diagrams of both processes are as illustrated in Figures 8 and 11.

The thermodynamic feature package is where the chemical compound information and calculation method are based on the selected chemical compound. This thermodynamic feature package contains equations of state (EOS), activity models and models dedicated to solving computational methods involving non-ideals in vapor and liquid mixtures. The package used is an extended non-random two-liquid (NRTL) package because this package is a package that uses an activity coefficient model that correlates with the activity coefficient of a compound with a mole fraction in the liquid phase.

3.1 Model Development and Simulation of Reactive Distillation Column

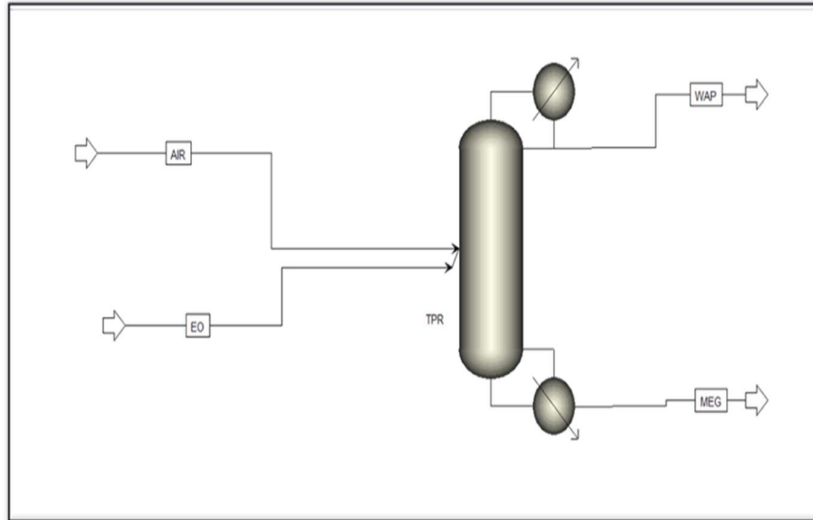


Figure 8. Reactive distillation column result using ASPEN Plus™

After developing the main process flow diagram, all parameter inputs were incorporated into each feed drain using an appropriate thermodynamic feature package to obtain the simulation results of Monoethylene Glycol production through a reactive distillation column. The 'AIR' line in figure 8 is the water feed drainage into the reactive distillation column while the 'EO' line is the Ethylene Oxide feed drainage into the reactive distillation column. For process output, 'WAP' line is the outflow of steam from the total condenser while 'MEG' line is the outlet which is the monoethylene glycol products. 'TPR' is a reactive distillation column using the RADFRAC method built into ASPEN Plus™.

Table 4. Output parameter for simulation production of MEG via RDC

Parameter	Value
Temperature	197.144°C
Pressure	1.01 bar
Liquid molar fraction	1
Vapor molar fraction	0
Molar enthalpy	-102.715 kcal/mol
Molar density	15.2887
Overall molar flowrate	26.3 kmol/hr
Overall Mass flowrate	1632.4 kg/hr
Overall Volumetric flowrate	1.72033 m ³ /hr

Table 5. Mole Fraction for every component in bottom product

Parameter	Value
Ethylene Oxide	5.08 x 10 ⁻¹³
Monoethylene Glycol	≈1
Water	2.79 x 10 ⁻¹¹

Based on Table 5, the mole fraction of monoethylene glycol for products from conventional processes is higher than 99% and approaching 1. Based on Weizhong An et. al. 2014, the objective of the reactive distillation column process is to achieve ethylene recovery greater than 99% and near -perfect water conversion.

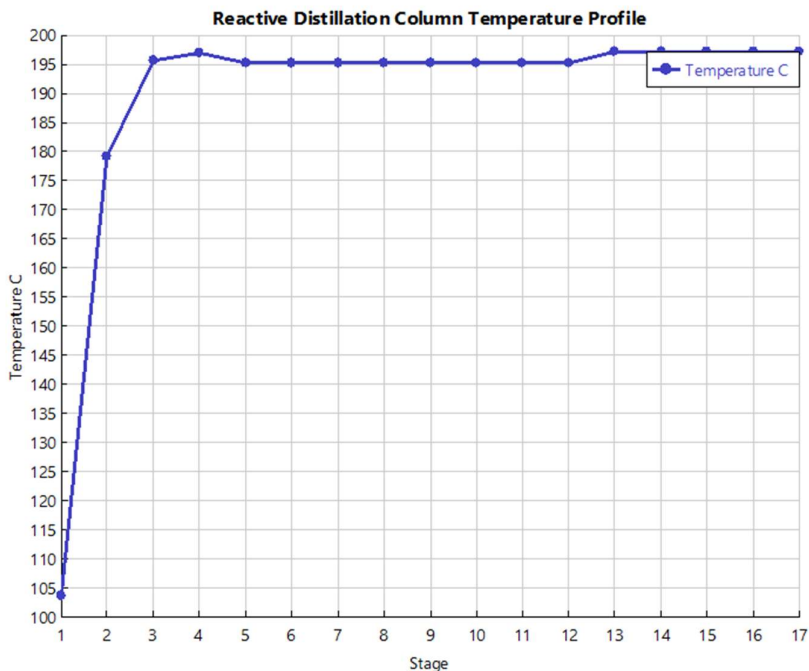


Figure 9. RDC temperature profile graph

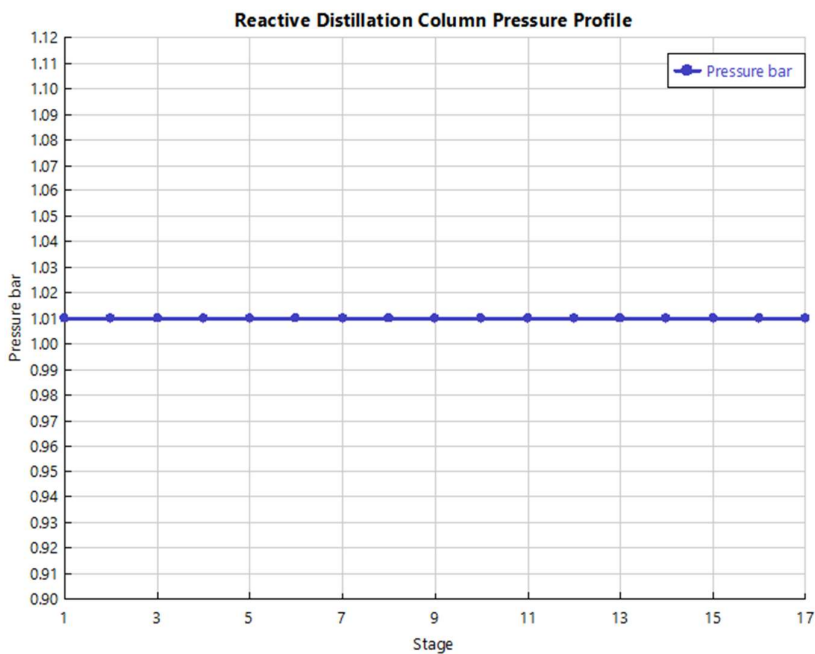


Figure 10. RDC pressure profile graph

Figure 9 shows the temperature profile inside each stage in the reactive distillation column for the production of Monoethylene Glycol. The temperature inside the reactive distillation column is the optimum temperature for

the ethylene oxide hydration reaction. The temperature range in the reactive distillation column plays an important role in the kinetics of the reaction. Since the reaction takes place in the liquid phase, the reaction temperature will approach the boiling point of monoethylene glycol. (Weizhong An et. Al. 2014)

Figure 10 shows a graph of the pressure profile against the level of the reactive distillation column. As can be seen in the graph, the pressure profile inside the reactive distillation column is fixed at 1.01 bar. The following are the optimum conditions for the ethylene oxide hydration process and also the results from the graph show that the established assumptions, where the pressure drop between the column plates can be negligible have been met. The reactive distillation column pressure is an important parameter in the reactive distillation process because the reactive distillation pressure will affect the relative volatility of the components in the process. (Weizhong An et al. 2014)

3.2 Model Development and Simulation of Conventional Process

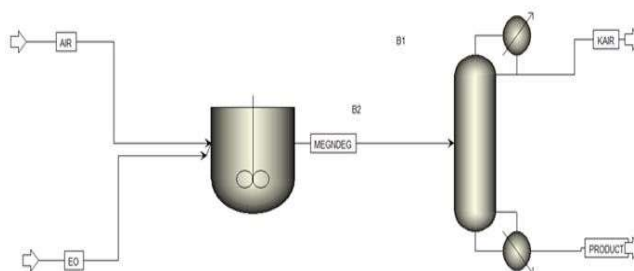


Figure 11. Conventional process simulation using ASPEN Plus™

To produce monoethylene glycol through a conventional process a continuous stirring tank reactor was selected to be used to develop simulations and modeling for this process. This process involves ethylene oxide and water being introduced into a continuous stirring tank reactor before proceeding with a distillation process involving two distillation columns. The first distillation column is to separate the resulting monoethylene glycol with water and the second distillation column is to separate monoethylene glycol and diethylene glycol. The process flow diagram is shown in Figure 11.

Based on the conventional process flow diagram, a model for the conventional process was developed using ASPEN Plus™. The thermodynamic packages used are NRTL and ELECNRTL. The 'WATER' channel in Figure 4.7 is the water feed drainage into the reactor while the 'EO' drainage is the feed drainage into the reactor. The reactor used is a reactor built into ASPEN Plus™ is using the RCSTR method. 'MEGNDEG' drainage is product drainage from the reactor before going through the dehydration process, 'KAIR' drainage containing water after the dehydration process while 'PRODUCT' drainage is Monoethylene Glycol and Diethylene Glycol drainage after the dehydration process.

Table 6. Output parameter 'MEGNDEG' reactor line for conventional process

Parameter	Value
Temperature	190 °C
Pressure	14.1855 bar
Liquid Molar Fraction	1
Vapor Molar Fraction	0
Molar Enthalpy	-102.66 kcal/mol
Molar Density	15.1445
Reactor Volume	42786.8 liter
Overall Molar flowrate	26.3 kmol/hr

Overall Mass flowrate	1686.59 kg/hr
Overall Volumetric flowrate	1.79313 m ³ /hr

Table 7. Output parameter for conventional process

Parameter	Value
Temperature	179.056 °C
Pressure	1 bar
Liquid Molar Fraction	1
Vapour Molar Fraction	0
Molar Enthalpy	-114.154 kcal/mol
Molar Density	12.756 kmol/m ³
Overall Molar flowrate	21.3 kmol/hr
Overall Mass flowrate	1596.51 kg/hr
Overall Volumetric Flowrate	1.66983/hr

Table 8. Final Result

Parameter	Value
Ethylene Oxide	5.40153 x 10 ⁻¹⁵
Monoethylene Glycol	0.575275
Water	0.066186
Diethylene Glycol	0.358607

Based on Table 8, the conversion of water is 0.93. The yield of monoethylene glycol is 0.57. Diethylene glycol is also formed in this process since the molar ratio of water is 1:1, the feed of water and ethylene oxide is set as constant variable to provide a legitimate comparison between the two processes.

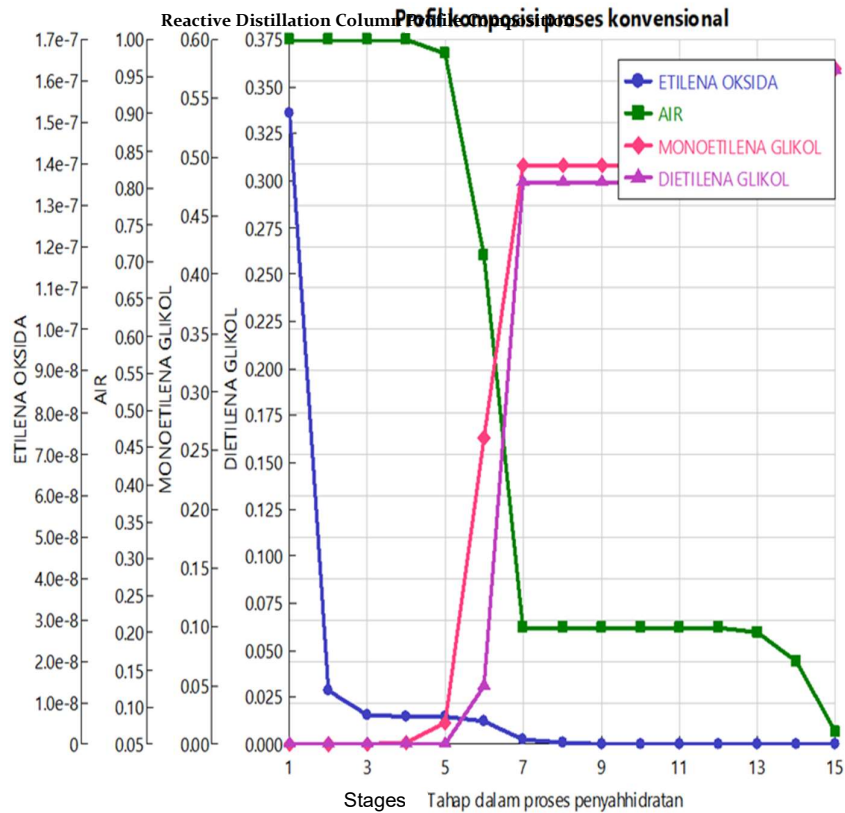


Figure 12. Composition profile for dehydration process in conventional process

Figure 12 shows the composition profile of each component in the dehydration process used in the conventional process. Ethylene oxide and water in the dehydration process are reduced due to the lower boiling point of the two components than Monoethylene Glycol and Diethylene Glycol. Conventional processes use excess water to avoid a reaction between Monoethylene Glycol and Ethylene Oxide to produce a homologous Diethylene Glycol. Water and Ethylene Oxide feeds were set as constant variables to indicate efficacy between conventional processes as well as processes using reactive distillation columns. Conventional processes that do not use a reactive distillation column are also unable to give preference towards the product because high homologues of Monoethylene Glycol such as diethylene glycol and triethylene glycol will be formed. Indirectly, the production rate of Monoethylene glycol will be affected and will not reach maximum production. (Lianghui Ding, 2019). **3.3 Process Analyses**

3.3.1 Conversion, Yield and Selectivity Analysis

Table 9. Comparison of water conversion and MEG yield for both process

Process	Water Conversion	Monoethylene Glycol Yield
Conventional Process	93%	57%
Reactive Distillation Column	>99%	>99%

The input parameters for the two processes were adjusted to obtain a comparison of effectiveness between the two processes. The results from the modeling and simulation get that the conventional process gives water conversion

of 93% while the reactive distillation head process gives water conversion of 99%. This is because the reactive distillation column process gives the maximum conversion rate by removing the continuously produced Monoethylene glycol directly giving an increase to the reaction kinetics and maximizing the chemical reaction that takes place. (Sakhre 2019)

In addition, the maximum water conversion and monoethylene glycol production higher than 99% are also due to the temperature profile in the reactive distillation column. The temperature profile plays an important role in controlling the kinetics of chemical reactions, since the reaction takes place in the liquid phase, the reaction temperature takes place in a temperature close to the boiling point of monoethylene glycol. (Weizhong An et. al. 2014)

By using water feed and ethylene oxide as constant variables, the efficiency of the reactive distillation column process is higher than the conventional process. In the conventional process, the water ratio will be higher than that of ethylene oxide to prevent the formation of high homologous monoethylene glycol. The water feed used in the 2001 Fulton Dye study used a water to ethylene oxide ratio of 10: 1 while in the Jackson 2018 study it used a water to ethylene oxide ratio of 20: 1. Ethylene oxide reacts more rapidly with monoethylene glycol than with water (Melhem et al. 2001), so without appropriate measures and controls, the reaction will usually produce a high homologue to monoethylene glycol. An important variable is the division of the ratio of water to monoethylene glycol to dilute the glycol solution and prevent high homologues from forming (Rebsdatt & Mayer 2005). In the conventional process modeling that has been done, the ratio of water to ethylene oxide used is 1:1, the formation of diethylene glycol has resulted in 35% which affects the production of monoethylene glycol in this process.

3.3.2 Process Efficiency Analysis

One of the methods used to see the effectiveness of the process is by using the process mass intensity method. This method looks at effectiveness by measuring the raw materials used and comparing them with the resulting product. The closer the process mass intensity value is to 1, the higher the process efficiency.

$$Process\ Mass\ Intensity = \frac{Raw\ Material\ Mass}{Product\ Mass} \quad (2)$$

Table 10. Process Mass Intensity(PMI) comparison.

Process	Weight of water in Feed	Weight of Ethylene Oxide in Feed	Weight of product	Process Mass Intensity Index
Conventional Process	495.96 kg	1212.78 kg	760.546 kg	2.15
Reactive Distillation Column	495.96 kg	1212.78 kg	1632.4 kg	1

As can be observed in Table 10, the process of producing monoethylene glycol via a reactive distillation column gives higher efficiency than the conventional process. This is due to, high water conversion, the selectivity of reaction is towards monoethylene glycol and also the high yield of monoethylene glycol that occurs in the reactive distillation column process. Reactive distillation column provides high conversion and recovery rates and directly offer high productivity to the process. The process mass intensity for the reactive distillation column is also lower than the conventional process. (Santaella 2005)

After modeling and simulating the reactive distillation column, the yield of monoethylene glycol and water conversion approached 1 or greater than 99%. The mass intensity of the process for the reactive distillation column

is also 1 where, the weight of the raw material used is the same as the weight of the resulting monoethylene glycol. This proves the effectiveness of the reactive distillation column process.

Table 11. Result comparison for reactive distillation column and conventional process

<i>Parameter</i>	<i>Conventional Process</i>	<i>Reactive Distillation Column</i>
Overall Mass Flowrate	1596.5 kg/hr	163.2 kg/hr
Water Conversion	93%	>99%
Monoethylene Glycol Yield	57%	>99%
Monoethylene Glycol Selectivity	0.57	~1
Process Mass Intensity	2.51	1

3.4 P&ID & Control Philosophy

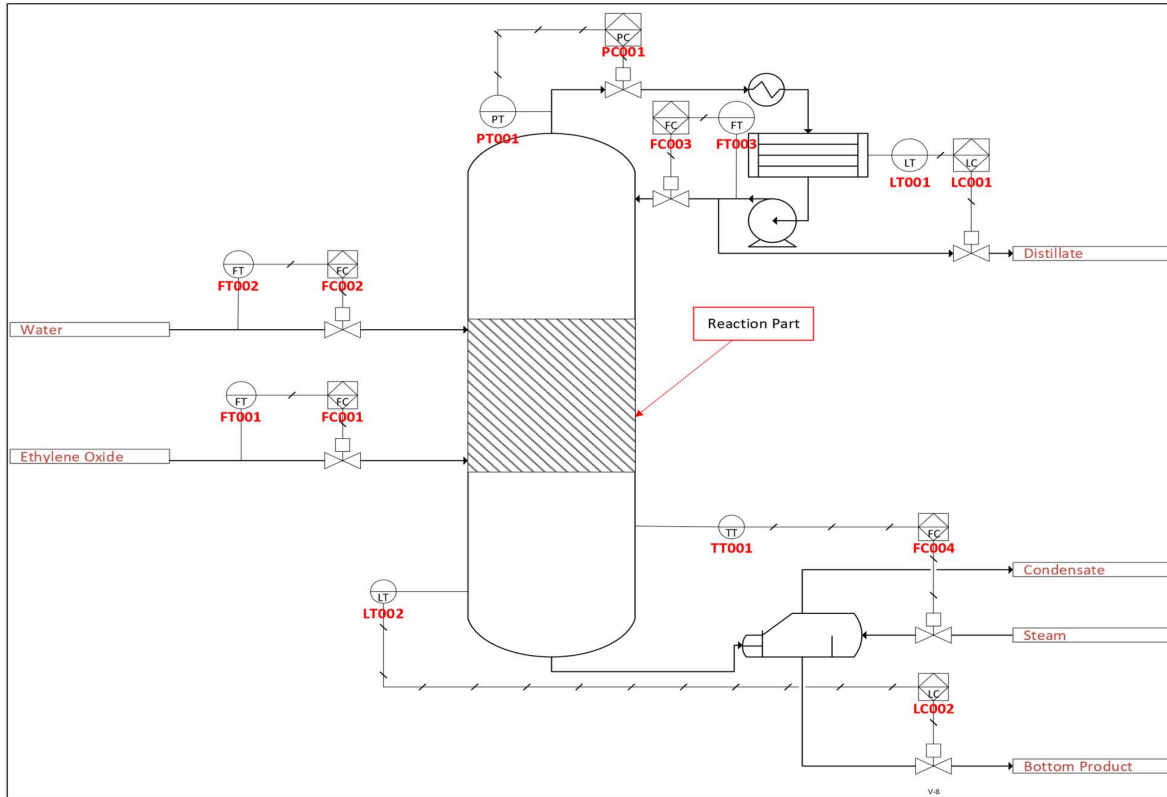


Figure 13: Basic engineering design of a control scheme for reactive distillation column

Figure 14 shows the high-level version of a control scheme for reactive distillation, to explain this in a simpler term is, this P&ID is the Basic Engineering Design phase, which moving forward this P&ID will be developed to greater details for the next phase. The control is shown HAZOP style, which is shown per every node, Distillate, Bottom, and Feed.

3.4.1 Feed Control

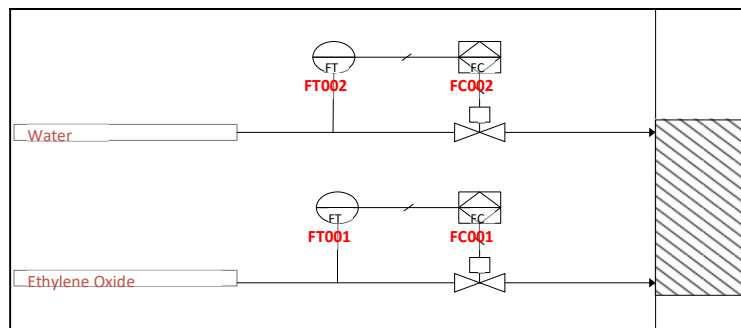


Figure 14: Control for Inlet of Reactive Distillation Column

For feed/input, this process requires adequate and meticulous control since the ratio of Ethylene Oxide to Water plays a part in this process. Hence FT, which is likely to be a flow transmitter will set the MOVs at Water inlet and Ethylene Oxide at fixed opening ratio and will be able to counter act any fluctuations in process.

3.4.2 Distillate Control

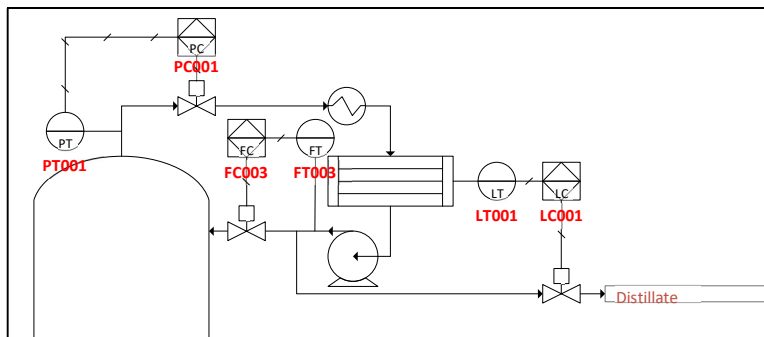


Figure 15: Control for Outlet (Distillate)

For distillate PT001 will detect the pressure in line going to the MOV at PC 001, which will then set the opening of MOV to dictate the percentage opening. A flow transmitter outside the reflux drum will then dictate the opening of MOV at FC003, that MOV is the return line where when the Flow is there the valve is set to a fixed opening. Once the level reaches a certain point, LT001 will send a signal to LC001 to open the MOV for distillate to flow through.

3.4.3 Bottom Control

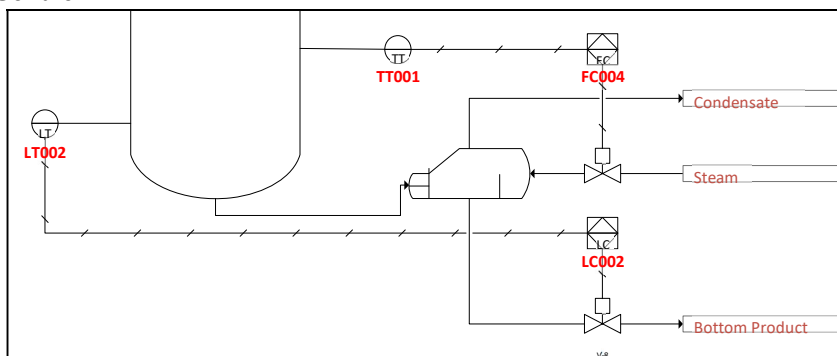


Figure 16: Control for Outlet (Bottom)

For bottom product, TT001 will then actively transmit the signal based on set temperature, if the temperature is lower than set temperature, MV for steam will be open and steam will be supplied to increase the overall system temperature. Based on the Level on the bottom of column, MOV for bottom product will open for MEG outlet.

5. Conclusions

The deliverables of this project have been completed where the development of models and simulations to produce MEG through reactive distillation column and the production of MEG through conventional processes have been carried out. These simulations were conducted using ASPEN Plus™ Version 11 software. Both simulations were conducted using the same molar flow rate feed to provide a clearer comparison. Analysis of both processes was also conducted. The analysis that has been conducted is an analysis using sustainability indicators.

Model development and simulation of MEG production through reactive distillation column and conventional process was carried out using ASPEN Plus™. Both processes use the NRTL thermodynamic package, to simulate reactions in the liquid state. Both processes use the same molar flow rate of feed to provide a clear comparison which is 26.3 kmol/hr of water and 27.53 kmol/hr of ethylene oxide. Monoethylene glycol yield for reactive distillation column is >99% while for conventional process is 57%.

The final objective is to look at the process effectiveness between the reactive distillation column process and the conventional process. Reactive distillation column gives a process mass intensity of 1 while conventional process is 2.15. The process mass intensity analysis shows that raw material is fully consumed and give the maximum amount of product so reactive distillation column is the more sustainable and effective process than conventional process.

There are a few recommendations for continuation for this process which is internal heat integration in the reactive distillation, process intensity and energy and cost savings when conduction reactive distillation calculation.

References

1. Abufares, A.A., Douglas, P.L., 1995. Mathematical modeling and simulation of an MTBE catalytic distillation process using speedup and
2. An, Weizhong, Zixin Lin, Jun Chen, and Jianmin Zhu. "Simulation and analysis of a reactive distillation column for removal of water from ethanol–water mixtures." *Industrial & Engineering Chemistry Research* 53, no. 14 (2014): 6056-6064.
3. Akpa, Jackson Gunorubon, and Paschal Onuorah. "SIMULATION AND CONTROL OF A REACTOR FOR THE NON-CATALYTIC HYDROLYSIS OF ETHYLENE OXIDE TO ETHYLENE GLYCOL." *SIMULATION* 8.2 (2018).
4. "ASPEN Tutorial | Chemical Engineering and Materials Science." 2021. Msu.edu. 2021. <https://www.chems.msu.edu/resources/tutorials/ASPEN>.
5. Batiha, Marwan M. "Dynamic Modelling of the Non-Catalytic Process of Ethylene Oxide Hydrolysis." *Journal of Science and Technology* 9 (2004).
6. Bamikole, J. O., and O. Taiwo. "MODELLING AND SIMULATION OF REACTIVE DISTILLATION SYSTEMS USING MATLAB AND ASPEN PLUS." *NSChE Journal* 33.1 (2018): 129-129.
7. Bamikole, J. O., and O. Taiwo. "MODELLING AND SIMULATION OF REACTIVE DISTILLATION SYSTEMS USING MATLAB AND ASPEN PLUS." *NSChE Journal* 33.1 (2018): 129-129.
8. Bartley, William J. *Process for the preparation of ethylene glycol*. No. US 4628129. 1986.
9. Budzinski, Kristi, Megan Blewis, Philip Dahlin, Daniel D'Aquila, Julia Esparza, Jack Gavin, Sa V. Ho et al. "Introduction of a process mass intensity metric for biologics." *New biotechnology* 49 (2019): 37-42.
10. Ding, Lianghui, et al. "Design and analysis of an intensified column with side reactor configuration for ethylene glycol production from ethylene oxide." *Chemical Engineering and Processing-Process Intensification* 147 (2020): 107744.
11. Dye, Robert Fulton. "Ethylene glycols technology." *Korean Journal of Chemical Engineering* 18, no. 5 (2001): 571579.
12. Fogler, Scott H. *Elements of Chemical Reaction Engineering*. 3rd ed. Englewood Cliffs, NJ: Prentice-Hall, 1998. Print.
13. Giwa, Saidat Olanipekun, Abel Adekanmi Adeyi, and Abdulwahab Giwa. "Application of model predictive control to renewable energy development via reactive distillation process." *International Journal of Engineering Research in Africa*. Vol. 27. Trans Tech Publications Ltd, 2016.
14. Giwa, Abdulwahab, Abel Adekanmi Adeyi, and Saidat Olanipekun Giwa. "Control of a reactive distillation process using model predictive control toolbox of MATLAB." *International Journal of Engineering Research in Africa*. Vol. 30. Trans Tech Publications Ltd, 2017.
15. Harmsen, G. Jan. "Reactive distillation: the front-runner of industrial process intensification: a full review of commercial applications, research, scale-up, design and operation." *Chemical Engineering and Processing: Process Intensification* 46, no. 9 (2007): 774-780.
16. Jackson, Jennifer R., and Ignacio E. Grossmann. "A disjunctive programming approach for the optimal design of reactive distillation columns." *Computers & Chemical Engineering* 25.11-12 (2001): 1661-1673.
17. K.L. Rock, CDTECH, "Selective hydrogenation of MAPD via catalytic distillation", in: ERTC Petrochemical Conference, Amsterdam, February 20-22, 2002
18. Kiss, Anton A., Megan Jobson, and Xin Gao. "Reactive distillation: stepping up to the next level of process intensification." *Industrial & Engineering Chemistry Research* 58.15 (2018): 5909-5918.
19. Kiss, Anton A. *Advanced distillation technologies: design, control and applications*. John Wiley & Sons, 2013.
20. National Institute for Occupational Safety and Health (NIOSH). *Pocket Guide to Chemical Hazards*. U.S. Department of Health and Human Services, Public Health Service, Centers for Disease Control and Prevention. Cincinnati, OH. 2015
21. Occupational Safety and Health Administration (OSHA). *Occupational Safety and Health Standards, Toxic and Hazardous Substances*. Code of Federal Regulations. 29 CFR 1910.1000. 1998.
22. Othmer, Donald F., and Mahesh S. Thakar. "Glycol production—hydration of ethylene oxide." *Industrial & Engineering Chemistry* 50, no. 9 (1958): 1235-1244.

23. Sakhre, Vandana. "Reactive Distillation: Modeling, Simulation, and Optimization." *Distillation-Modelling, Simulation and Optimization*. IntechOpen, 2019.
24. Silva, R. J. M. C. L., et al. "Ethanollic Biodiesel Production: A Comparative Study between a Plug Flow Reactor and Reactive Distillation." *Brazilian Journal of Chemical Engineering* 34.3 (2017): 811-819.