

## Improving Product Purity of Ethylene Glycol Production from Ethylene Oxide by Modify Process Using Multi-stage Distillation

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### Abstract

Ethylene glycol (EG) is an important industrial chemical widely used in the manufacture of polyester fibers, antifreeze formulations, and heat-transfer fluids. Industrially, EG is produced through the hydration of ethylene oxide; however, achieving high product purity remains a significant challenge due to the presence of water and higher glycols in the reaction mixture. This study proposes a process modification aimed at improving ethylene glycol purity through the implementation of a multi-stage distillation system. The conventional single-stage distillation configuration was evaluated and compared with a modified two-stage distillation scheme. Simulation results indicate that the proposed modification significantly enhances separation performance, increasing ethylene glycol mole fraction from 0.8991 in the unmodified process to 0.9990 in the modified configuration. The improvement is attributed to better distribution of separation duties and enhanced control of vapor–liquid equilibrium across multiple distillation stages. These findings demonstrate that multi-stage distillation, supported by rigorous process simulation, is an effective strategy for producing high-purity ethylene glycol and offers valuable insights for industrial process optimization and design.

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**Keywords:** Ethylene glycol; Ethylene oxide; Multi-stage distillation; Process simulation; Product purity

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### 1. Introduction

Ethylene glycol (EG) is an essential chemical widely utilized in the production of polyester fibers, antifreeze formulations, heat-transfer fluids, and various industrial solvents [1]. Industrially, EG is primarily produced through the hydration of ethylene oxide (EO), a reaction that generates monoethylene glycol (MEG) as the main product along with diethylene glycol (DEG) and triethylene glycol (TEG) as secondary byproducts [2]. The downstream purification stage plays a critical role in ensuring that EG meets the high purity specifications required for industrial applications [3]. However, the purification process is challenging due to the high boiling point and complex thermophysical

properties of EG, which demand efficient and well-designed separation systems [1]. As a result, improving the efficiency and performance of EG purification remains a central focus in modern chemical process development.

In industrial practice, EG purification is commonly performed using fractional distillation, which can handle the narrow volatility differences between EG and its associated by-products [3]. Conventional single-column distillation often requires many stages and high reflux ratios to achieve the desired purity, leading to significant energy consumption [4]. To address these limitations, various alternative approaches such as extractive distillation, heterogeneous distillation, and optimization-based process design have been proposed to enhance separation efficiency in complex glycol systems [5]. Recent studies also highlight the importance of process

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simulation tools, such as Aspen HYSYS, in evaluating separation performance and identifying opportunities for process intensification [2]. These advancements underscore the need for innovative distillation configurations that can deliver higher purity with improved energy efficiency.

Given the increasing demand for high-purity EG, modified distillation configurations have emerged as promising strategies to enhance purification performance. Multi-stage distillation has demonstrated the ability to improve separation efficiency by distributing the purification load across multiple columns operating under optimized conditions [6]. This configuration enables more precise control of vapor-liquid equilibrium behavior, facilitating the separation of components with close boiling characteristics [7]. Studies on process intensification further indicate that increasing the number of stages and optimizing operating parameters can significantly improve EG purity without proportionally increasing energy requirements [1]. Additionally, sustainable process design principles emphasize the importance of integrating efficient separation technologies to enhance overall process performance in the chemical industry [8]. Therefore, modifying the EG purification process through multi-stage distillation represents a strategic pathway to achieve superior product quality and operational efficiency.

In this context, the present study proposes the implementation of a two-stage distillation system to improve the purity of ethylene glycol, supported by rigorous simulation and process modification using Aspen HYSYS [1]. This modification aims to achieve higher EG purity compared to the conventional single-column configuration by distributing the separation duty across two optimized distillation units [4]. The application of a two-stage distillation approach is expected to enhance separation efficiency and improve the quality of the final EG product [5]. Furthermore, simulation-based evaluation enables systematic optimization of operating conditions and column design to achieve improved performance [2]. Ultimately, the findings of this study are expected to contribute to advancing chemical process design principles that balance efficiency, sustainability, and industrial feasibility [8].

## 2. Methods

### 2.1 Process Simulator Tool

The material for this work includes ethylene oxide, process water, ASPEN HYSYS V.11.0, reactor, distillation column and centrifugal pump. In this simulation of the production ethylene

glycol process the UNIQUAC property package was employed [9].

### 2.2. Yield Optimization using Heat Exchanger as Independent Variable

A distillation column is a widely used separation unit in the chemical industry, operating on the principle that different components in a mixture have different boiling points. Heat is supplied at the bottom of the column through a reboiler, generating vapor that rises through the stages. At the top, a condenser cools the overhead vapor into liquid, which is collected in a reflux drum. Part of this liquid is returned to the column as reflux to enhance separation efficiency, while the remainder is withdrawn as distillate [10].

Distillation separates mixtures based on significant differences in boiling point and vapor pressure. Within the column, the vapor and liquid phases continuously contact each other and reach equilibrium, creating distinct composition gradients. Components with lower boiling points (higher vapor pressures) preferentially enter the vapor phase, while those with higher boiling points remain in the liquid phase. This counter-current mass transfer makes the distillation column a critical and complex piece of equipment for separation and purification processes [11]. The calculation of yield can be seen in Equation (1) [12].

$$Purity_{EG}(\%) = \frac{x_{EG}}{x_{EG} + x_{DEG} + x_{Water}} \times 100\% \quad (1)$$

In this study, distillation is employed to increase the purity of ethylene glycol. Prior to installing a second distillation column, the product purity was 89.91% with a water content of 10.01%. By adding the additional column, the separation performance improved significantly, resulting in an ethylene glycol purity of 99.90% with no detectable water content.

## 3. Results and Discussion

### 3.1. Basic Process Flow Diagram of Ethylene Glycol Production

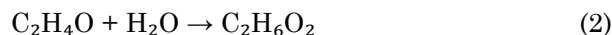
The basic (unmodified) process flow diagram for ethylene glycol production is shown in Figure 1, while the corresponding Aspen HYSYS process simulation is presented in Figure 2. The process begins with ethylene oxide as the primary feedstock. The feed is pumped from the storage tank, increasing its pressure from 1 atm to 13 atm. The pressurized stream leaving the pump is designated as Stream 1 (S1). S1 is then directed to the reactor, where the hydration reactions occur. Upon completion of the reactions, the reactor effluent consists of both vapor and liquid phases.

The vapor phase contains no ethylene glycol (EG), diethylene glycol (DEG), or water. The liquid phase, however, contains predominantly EG, a smaller fraction of DEG, and a large amount of water. This liquid product stream is subsequently fed to an atmospheric distillation column, where EG, DEG, and water are separated based on their boiling point differences.

### 3.2. Thermodynamic Review

The objective of this thermodynamic analysis is to apply the Gibbs equation ( $G = H - T.S$ ) to predict the spontaneity of chemical processes under specified operating conditions [14]. In addition, the analysis aims to identify whether the reaction proceeds exothermically or endothermically and to evaluate its potential reversibility [15]. The thermodynamic model incorporates empirical correlations and equations of state to estimate essential properties, including enthalpy, entropy, and heat capacity. Evaluating reaction thermodynamics through the standard enthalpy change ( $\Delta H^{\circ}_{298K}$ ) provides a critical foundation for managing energy requirements and optimizing process performance. Furthermore, assessing reaction reversibility using the standard Gibbs free energy ( $\Delta G^{\circ}_{298K}$ ) enables the determination of reaction feasibility and the system's inherent tendency to reach equilibrium under defined conditions [16]. Thermodynamic modelling also predicts equilibrium product distributions, phase behaviour, and overall energy demand, thereby supporting the design of efficient and sustainable chemical processes by informing the selection of operational parameters that maximize reaction yields while minimizing energy consumption. In this context, the values of  $\Delta H_f^{\circ}$  and  $\Delta G_f^{\circ}$  serve as key indicators for characterizing reaction

energetics and guiding process optimization [17]. The value of  $\Delta H_f^{\circ}$  and  $\Delta G_f^{\circ}$  can be seen in Table 1. The chemical reaction for producing ethylene glycol can be described as follows:



Standard heat of reaction at 298K ( $\Delta H^{\circ}_{298K}$ ):

$$\Delta H^{\circ}_{298K} = \sum \Delta H_f^{\circ} \text{ product} - \sum \Delta H_f^{\circ} \text{ reactant}$$

$$\Delta H^{\circ}_{298K} = (\Delta H_f^{\circ} C_2H_6O_2) - (\Delta H_f^{\circ} C_2H_4O + \Delta H_f^{\circ} H_2O) = -93.1 \text{ kJ/mol}$$

Based on the calculations, the result is negative enthalpy change, indicating that the reaction is exothermic.

$\Delta G^{\circ}_{298K} = \sum \Delta G_f^{\circ} \text{ product} - \sum \Delta G_f^{\circ} \text{ reactant}$

$$\Delta G^{\circ}_{298K} = (\Delta G_f^{\circ} C_2H_6O_2) - (\Delta G_f^{\circ} C_2H_4O + \Delta G_f^{\circ} H_2O) = -168.6 \text{ kJ/mol}$$

Equilibrium constant ( $K_2$ ) in the standard state:

$$\Delta G^{\circ}_{298K} = -RT \ln K$$

$$\ln K_2 = - \frac{\Delta G^{\circ}_{298K}}{RT} = 68.04$$

$$K_2 = 1.6 \times 10^{29}$$

Equilibrium constant ( $K_1$ ) at reactor temperature  $T = 190 \text{ }^{\circ}\text{C}$ :

$$\ln \frac{K_1}{K_{298}} = \frac{-\Delta H_{298}}{R} \left( \frac{1}{T} - \frac{1}{T_{298}} \right)$$

$$\ln \frac{K_1}{1.6 \times 10^{29}} = \frac{93.1 \text{ kJ}}{0.008314 \frac{\text{kJ}}{\text{mol}}} \left( \frac{1}{463} - \frac{1}{298} \right)$$

$$K_1 = 2.5 \times 10^{23}$$

Due to the low equilibrium constant, the ethylene glycol reaction is irreversible.

Table 1. The value of  $\Delta H_f^{\circ}$  and  $\Delta G_f^{\circ}$  of compound.

Compound	Molecular Formula	$\Delta H_f^{\circ}$ (kJ/mol)	$\Delta G_f^{\circ}$ (kJ/mol)
Ethylene Oxide	$C_2H_4O$	-52.6	-13.2
Water	$H_2O$	-241.8	-237.1
Ethylene Glycol	$C_2H_6O_2$	-387.5	-418.9
Di-ethylene Glycol	$C_4H_{10}O_2$	-571.2	-409

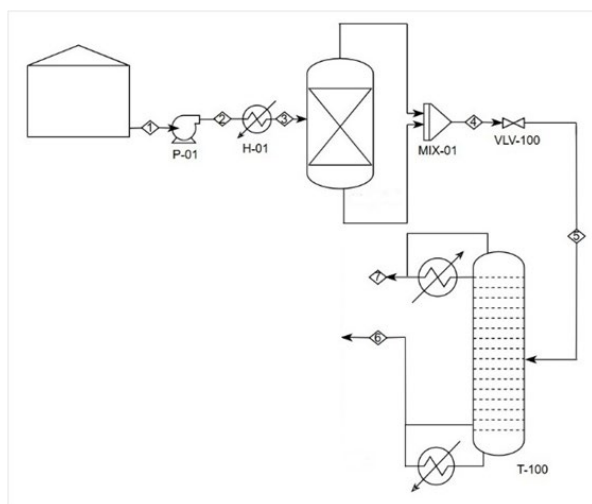


Figure 1. Unmodified process flow diagram (PFD) to be simulated.

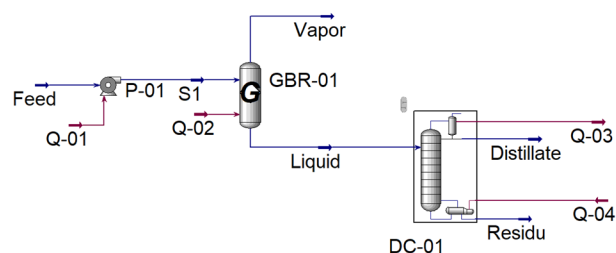


Figure 2. Process simulation of the unmodified/basic process using Aspen HYSYS [13].

### 3.3. Improvement of Product Purity Due to the Process Modifications

The quality of ethylene glycol products acts as a benchmark for assessing both the factory's performance and the overall standard of manufactured products. Greater product purity reflects enhanced quality in the product and the factory [18]. To evaluate the percentage purity in the two simulated processes, calculations were performed using Equation (1). The mass of the ethylene glycol product and mole fraction mass were derived from Aspen HYSYS data. Table 2 provides the data for the total product mole fraction in the unmodified process design.

Simulation constitutes a critical tool for evaluating the performance of the modified the purity level of the hydrochlorination process, which produces ethylene glycol as the main product, is an important indicator of the overall quality of the product produced. Purity is a product yield that is devoid of impurities, contaminants, and foreign matter of any kind [19]. The percentage purity is calculated based on the product mole fraction and total mole fraction values obtained from Aspen HYSYS data. The total mole fraction data in the basic process design can be seen in Table 2. Using the data in Table 2, the purity of ethylene glycol can be calculated using Equation (1).

$$\text{Purity}_{\text{EG}}(\%) = \frac{x_{\text{EG}}}{x_{\text{EG}} + x_{\text{DEG}} + x_{\text{Water}}} \times 100\% = 89.91\%$$

Based on the calculation, the main product ethylene glycol using the basic process produces a purity percentage of 89.91%. To compare with the modified process, the total mole fraction data on the modified process design can be seen in Table 2. Using the data in Table 2, the purity of ethylene glycol can be calculated using Equation (1).

$$\text{Purity}_{\text{EG}}(\%) = \frac{x_{\text{EG}}}{x_{\text{EG}} + x_{\text{DEG}} + x_{\text{Water}}} \times 100\% = 99.90\%$$

Based on the calculation, the main product of methyl ethylene glycol the modified process produces a purity percentage of 99.90%.

Table 2. Difference of Ethylene Glycol mole fraction obtained from basic process and modified process.

Process	Mole fraction of Ethylene Glycol	Mole fraction of Water	Mole fraction of Diethylene Glycol
Basic	0.8991	0.1001	0.0008
Modified	0.9990	0.0000	0.0010

### 4. Conclusion

Based on the data obtained from the observations conducted, prior to modification the ethylene glycol product purity was 0.8991. After the process modification, the purity increased significantly to 0.9990, indicating a substantial improvement in product quality. This enhancement was achieved through process modifications implemented in the ethylene glycol production system, and the results presented in this paper are expected to serve as a foundation for further studies on improving product purity and optimizing separation performance in industrial ethylene glycol applications.

### Credit Author Statement

Author Contributions: M.A. Nailendra: Conceptualization, Methodology, Investigation, Software, Visualization, Writing, Review & Editing, Supervision; M.R. Wijaya: Conceptualization, Investigation, Software, Visualization, Writing; R.C. Pangabean: Conceptualization, Methodology, Formal Analysis, Resources, Validation, Writing; T. Rifansyah: Conceptualization, Visualization,

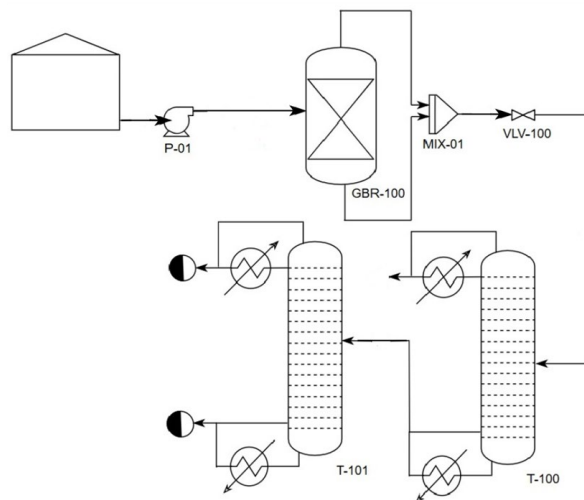


Figure 3. Modified process flow diagram to be simulated.

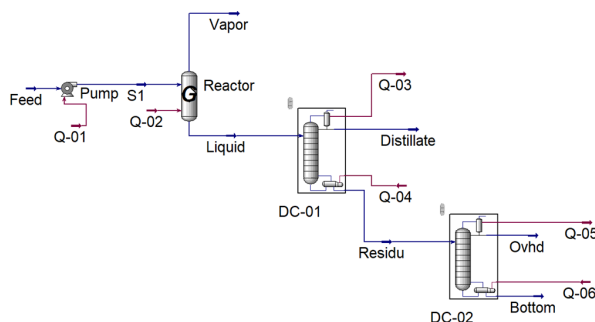


Figure 4. Modified/basic process flow diagram from Aspen HYSYS simulation.

Methodology, Investigation, Resources, Data Curation, Writing; Y.L Halimah: Conceptualization, Methodology, Writing, Review & Editing, Project Administration, Validation. All authors have read and agreed to the published version of the manuscript.

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