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# Assessment of Reactor Efficiency and Yield in Ethylenediamine Synthesis: A Case Study Utilizing Heterogeneous Catalysis

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***Abstract*—This research focuses on enhancing the production of ethylenediamine (EDA) through the catalytic reaction of monoethanolamine (MEA) and ammonia ($NH_3$) in a heterogeneous plug flow reactor (PFR) using Aspen HYSYS simulation. The process involves a primary reaction converting MEA to EDA and a secondary reaction yielding diethylenetriamine (DETA) as a byproduct. Raney Nickel serves as the catalyst, while key operational parameters—temperature, pressure, and feed ratios—are systematically adjusted to evaluate their impact on yield, selectivity, and conversion efficiency. The study identified optimal conditions for achieving a maximum EDA yield of 94.4% at 150°C, 6000 kPa, and a 14:1 ammonia-to-MEA molar ratio, effectively minimizing byproduct formation. The findings underscore the effectiveness of Aspen HYSYS as a tool for simulating and optimizing complex chemical processes, providing critical insights into reactor design and operational control. Sensitivity analyses reveal increased pressure improves conversion rates, while lower temperatures enhance EDA selectivity over DETA formation. These insights advance the understanding of heterogeneous catalytic processes and offer strategies for improving EDA production efficiency on an industrial scale. In addition to promoting sustainable chemical manufacturing, the results offer practical recommendations for minimizing environmental impact and optimizing process efficiency. Future efforts should prioritize experimental validation, explore alternative catalysts, and investigate innovative reactor designs to further refine and scale up the production of EDA, aligning with industrial and environmental goals.**

***Keywords*— Ethylenediamine; Monoethanolamine; plug flow reactor; simulation; HYSYS.**

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## I. INTRODUCTION

Ethylenediamine (EDA) is a multifunctional compound that finds widespread application in the synthesis of chelating agents, pharmaceuticals, and polymeric materials [1]-[8]. The increasing global demand for EDA has prompted significant research into optimizing its synthesis to improve yield, efficiency, and sustainability [9]-[12]. Among the available methods for producing EDA, the reductive amination of *monoethanolamine* (MEA) with ammonia, catalyzed by heterogeneous materials like Raney Nickel, has emerged as a promising pathway due to its simplicity and efficiency.

At present, there are three main techniques utilized for the synthesis of ethylene amines. The first method involves the reaction of ethylene *dichloride* with *ammonia*, resulting in a comprehensive array of *ethyleneamine* products. The second method is the reductive amination of *monoethanolamine*, which predominantly yields lighter ethylene amines such as ethylenediamine (EDA). Lastly, the catalytic reaction between *Monoethanolamine* (MEA) and Ethylenediamine facilitates the production of higher-order *ethylene amines* [13]-[16]. Kinetic constants for the production of Ethylenediamine are accessible [17], [18].

This work aims to investigate the reductive amination of *Monoethanolamine* (MEA) with Ammonia ($NH_3$) under a heterogeneous catalyst (referred to as the "RA Process"). Figures 1 and 2 illustrate the typical production of ethylenediamine (EDA) through the RA process [19]. The recommended catalysts for this procedure are Raney nickel or cobalt, copper, modernity, chromite, platinum, osmium, palladium, and others [9], [20]-[23].

In recent years, attention has switched towards improving reactor design and operating conditions to optimize yield while minimizing byproduct formation [3], [24]-[26]. The synthesis of EDA is a complicated process that involves both primary and secondary reactions. The primary response transforms MEA to EDA, while the secondary reaction yields

Diethylenetriamine (DETA), an undesirable byproduct. Controlling operating variables such as temperature, pressure, and catalyst characteristics is critical for increasing EDA selectivity while reducing DETA production.

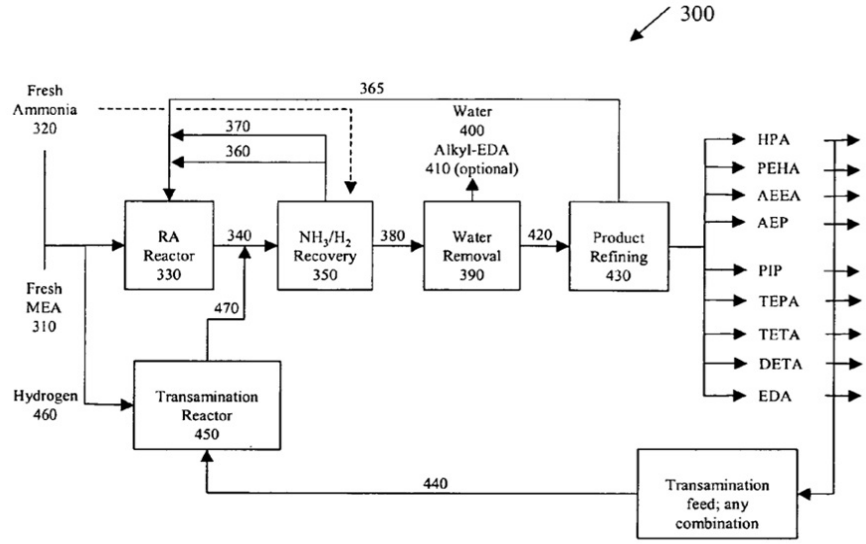


Fig. 1 Flowchart of Ethylenediamine Production, Source: [19].

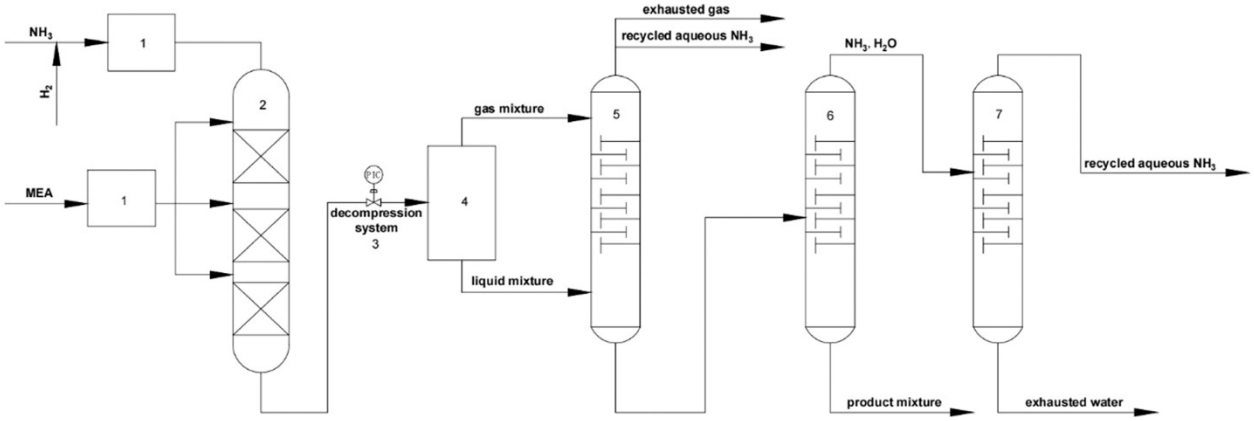


Fig. 2 Schematic diagram of the apparatus: 1, heater; 2, reactor; 3, valve; 4, gas separator; 5–7, distillation column. Source: [9].

The Plug Flow Reactor (PFR) is commonly employed for heterogeneous catalytic reactions, including EDA production, due to its ability to sustain high conversion rates, manage heat transfer effectively, and enable precise control over reaction kinetics [27]-[32]. However, optimizing PFR performance for EDA production remains a complex challenge. This is primarily because synthesis involves primary reactions to produce EDA and secondary reactions that generate byproducts such as diethylenetriamine (DETA), which reduce process selectivity and economic efficiency. Effective reactor design and operational optimization are critical for enhancing EDA yield and minimizing byproduct formation.

Fluid dynamics, reactor size, and catalyst activity are some of the variables that affect PFR performance in heterogeneous catalysis. Numerous studies have examined optimizing PFRs for various chemical processes, emphasizing how crucial reactor design is to attaining high yield and selectivity.

Several studies have explored the chemistry and catalysis involved in EDA production [9], [33], [34]. For instance, Ma et al. [21] analyzed the effects of Ni particle size on the amination of MEA, and Xie et al. [22] compared the catalytic efficiency of nickel and cobalt for similar processes. While these studies have contributed valuable insights into catalytic behavior, they often focus on catalyst performance rather than the holistic optimization of the production process. Similarly, research on PFR applications has examined general principles of reactor performance but lacks targeted analyses for EDA synthesis. The interactions among critical parameters, such as temperature, pressure, and feedstock ratios, and their combined impact on yield and selectivity remain underexplored.

Simulation tools like Aspen HYSYS have been widely used in the chemical industry for process design and optimization due to their robust capabilities in modeling complex reaction systems [35]-[45]. However, their application to optimize PFR performance for EDA production is not well-documented in existing literature. This represents a significant gap in leveraging advanced simulation to improve EDA's industrial-scale production efficiency. Aspen HYSYS advanced thermodynamic packages, reaction kinetics modeling, and sensitivity analysis tools make it ideal for studying heterogeneous catalytic processes like EDA synthesis [46]-[48]. This research uses Aspen HYSYS to evaluate the trade-offs between operating conditions, product yield, and byproduct formation, offering a practical approach to achieving optimal reactor performance. This study aims to address these gaps by evaluating the performance of a PFR in

EDA production through detailed simulations using Aspen HYSYS. The research systematically investigates the impact of key operational parameters—including temperature, pressure, and the ammonia-to-MEA feed ratio—on reactor performance, with the goal of maximizing EDA yield and minimizing DETA formation.

The novelty of this research lies in its integration of advanced simulation tools to analyze and optimize the EDA synthesis process. By conducting a comprehensive sensitivity analysis and identifying optimal reactor conditions, this study advances knowledge in reactor design and process control and offers actionable insights for improving the scalability and sustainability of EDA production.

## II. Materials and Method

### A. Chemicals and Catalysts

In this study, Ethylenediamine (EDA) is produced through the catalytic reaction of *Monoethanolamine* (MEA) with Ammonia ($NH_3$). Raney Nickel, a catalyst known for its high activity and stability in hydrogenation reactions, is employed in this process. Raney Nickel is crucial for enhancing the conversion of MEA to EDA while reducing the formation of by-products like diethylenetriamine (DETA).

### B. Simulation Setup

The process simulation was conducted utilizing Aspen HYSYS V14, a process modeling software extensively employed in the chemical industry for dynamic and steady-state simulations. This software was selected due to its comprehensive thermodynamic package and ability to model complex chemical reactions accurately.

### C. Reactor Model

The reactor used in the simulation is a plug flow reactor (PFR), which is suitable for heterogeneous catalytic processes. The PFR model in HYSYS was chosen because of its ability to handle variations in concentration and temperature along the reactor length, providing a more accurate representation of industrial reactor conditions.

### D. Thermodynamic Package

The NRTL equation of state was employed as the thermodynamic package to calculate the system's phase equilibria and thermodynamic properties. This equation of state is appropriate for the high-pressure systems typically involved in EDA production.

### E. Reaction Kinetics

The primary reaction modeled in the simulation is the conversion of MEA to EDA, which the following reaction can represent:

$$NH_3 + C_2H_7NO \rightarrow C_2H_4(NH_2)_2 + H_2O$$

or

$$Ammonia + MEA \rightarrow EDA + Water$$

The secondary reaction, which leads to the formation of DETA, was also included in the model:

$$C_2H_7NO + C_2H_4(NH_2)_2 \rightarrow C_4H_{13}N_3 + H_2O$$

or

$$MEA + EDA \rightarrow DETA + Water$$

The reaction kinetics were defined using rate expressions based on literature values (Table 1), with the activation energy and pre-exponential factors for both reactions taken from relevant studies.

### F. Operating Conditions

The simulation was conducted under various operating conditions to identify the optimal parameters for maximizing EDA yield. The key parameters varied include (1) Temperature (the reactor temperature was varied between 150°C and 250°C to assess its impact on the reaction rate and product distribution), (2) Pressure (the pressure within the reactor was adjusted from 2000 kPa to 6000 kPa to evaluate its influence on the reaction equilibrium and conversion rates), (3) $NH_3$ to MEA ratio was modified to study its effect on the overall reaction rate and selectivity.

### G. Data Analysis

The output data from the HYSYS simulation, including the molar flow rates of EDA, MEA, and byproducts, were analyzed to determine the yield and conversion rates. Sensitivity analyses were performed to understand each parameter's influence on EDA production. Graphs and tables were generated to present the relationship between the operating conditions and the reactor performance.

### H. Optimization Procedure

A systematic approach was used to optimize the reactor conditions. Initially, a baseline simulation was conducted using standard operating conditions derived from industrial practices. Following this, individual parameters were varied systematically to observe their impact on the yield and selectivity. The optimal conditions were identified based on the highest EDA yield with minimal byproduct formation.

### I. Block Diagram

The block diagram for this process is shown in Figure 3. The figure represents a Plug Flow Reactor (PFR-100), a chemical reactor used for continuous processing. MEA (*Monoethanolamine*) and Ammonia are fed into the reactor. Two streams exit the reactor—one labeled "Products," representing the desired chemical outcome, and another labeled "Q," referring to heat transfer to maintain the reactor temperature at isothermal conditions. This setup is commonly used in chemical engineering to ensure efficient reaction progression by allowing reactants to move through the reactor in a streamlined, sequential manner.

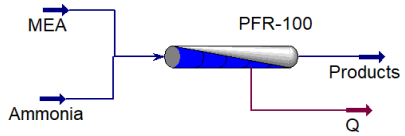


Fig. 3 HYSYS Process Flow Diagram for Ethylenediamine Production in Plug Flow Reactor

## III. Results and Discussion

### A. Simulation Outcomes

The Aspen HYSYS simulation provided comprehensive insights into ethylenediamine (EDA) production under varying reactor conditions. The molar flow rates of EDA,

unreacted *monoethanolamine* (MEA), ammonia ($NH_3$), and the byproduct diethylenetriamine (DETA) were analyzed. As the simulation explored changes in temperature, pressure, and the ratio of ammonia to *monoethanolamine*, key trends emerged regarding the yield and selectivity of the reactions. Table 1 provides the basis for the simulation.

TABLE 1
BASIS CONDITION FOR SIMULATION

| Variable | Value, Unit |
|---|---|
| $T_{operating}$ | 150°C to 250°C |
| $P_{operating}$ | 2000 kPa to 6000 kPa |
| $A_1$ (main reaction) | 5.1271 x $10^5$ kg mole/$m^3$.h |
| $E_1$ (main reaction) | 14200 kJ/kg mole |
| $A_2$ (side reaction) | 3.4321 x $10^5$ kgmole/$m^3$.h |
| $E_2$ (side reaction) | 11300 kJ/kg mole |
| Molar flow MEA inlet | 4000 kg mole/h |
| Molar flow Ammonia inlet | 10000 kg mole/h |
| Raney catalyst density | 6500 kg/$m^3$ |
| Raney catalyst sphericity | 1 |
| Type of reactor | Plug Flow Reactor (PFR) |
| Number of segments | 20 |
| Length | 12 m |
| Diameter of reactor | 6 m |
| Void fraction | 0.1 |

## B. *Temperature Effect*

The temperature range between 150°C and 250°C was systematically explored. It was observed that, while higher temperatures typically increase reaction rates, the yield of EDA peaked at around 150°C. Beyond this point, increasing the temperature reduced yield due to increased byproduct formation, particularly DETA (see Figs 4, 5, and Table 2). This behavior suggests that a balance must be maintained between maximizing conversion rates and suppressing unwanted side reactions.

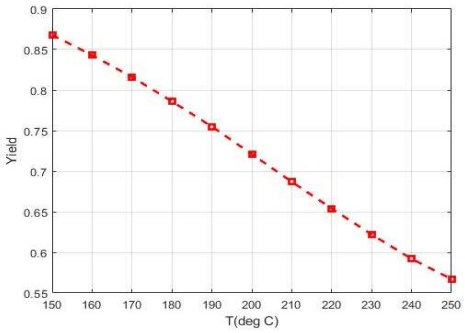


Fig. 4 Yield vs Temperature at 2000 kPa

Compared to previous studies by Maxwell [49], the results align with observations that lower temperatures favor selectivity towards lighter *ethylene-amines* like EDA. The simulations revealed that an optimal yield of 86.8% was achieved at 150°C and 2000 kPa, confirming the significant role temperature plays in reaction optimization [49].

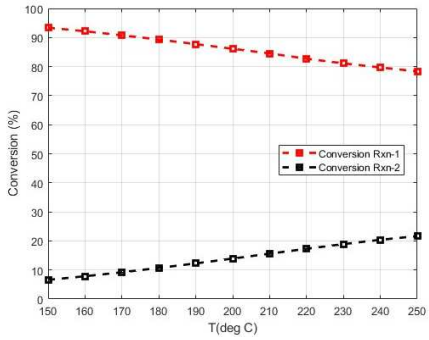


Fig. 5 Conversion vs Temperature at 2000 kPa

TABLE II
EFFECT OF TEMPERATURE

| T (°C) | P (kPa) | MEA inlet (kg mole/h) | NH3 inlet (kg mole/h) | Product (kg mole/h) | EDA in Product (kg mole/h) | $NH_3$ excess (kg mole/h) | Yield | DETA in Product (kg mole/h) |
|---|---|---|---|---|---|---|---|---|
| 150 | 2000 | 4000 | 10000 | 14000 | 3472.000 | 6263.600 | 0.868 | 263.200 |
| 160 | 2000 | 4000 | 10000 | 14000 | 3372.600 | 6314.000 | 0.843 | 313.600 |
| 170 | 2000 | 4000 | 10000 | 14000 | 3262.000 | 6368.600 | 0.816 | 368.200 |
| 180 | 2000 | 4000 | 10000 | 14000 | 3144.400 | 6427.400 | 0.786 | 428.400 |
| 190 | 2000 | 4000 | 10000 | 14000 | 3018.400 | 6490.400 | 0.755 | 491.400 |
| 200 | 2000 | 4000 | 10000 | 14000 | 2885.400 | 6557.600 | 0.721 | 557.200 |
| 210 | 2000 | 4000 | 10000 | 14000 | 2749.600 | 6624.800 | 0.687 | 624.400 |
| 220 | 2000 | 4000 | 10000 | 14000 | 2616.600 | 6692.000 | 0.654 | 691.600 |
| 230 | 2000 | 4000 | 10000 | 14000 | 2486.400 | 6756.400 | 0.622 | 756.000 |
| 240 | 2000 | 4000 | 10000 | 14000 | 2368.800 | 6815.200 | 0.592 | 814.800 |
| 250 | 2000 | 4000 | 10000 | 14000 | 2266.600 | 6867.000 | 0.567 | 866.600 |

## C. *Pressure Effect*

Pressure also significantly influences the reaction kinetics and yield. As the reactor pressure increased from 2000 kPa to 6000 kPa, the yield of EDA rose steadily, peaking at 94.4% at 6000 kPa (Table 3, Figs. 6 and 7). This increase is attributed to the positive effect of pressure on shifting the equilibrium towards product formation, as per Le Chatelier's principle. These findings are consistent with existing literature on pressure optimization in amination reactions.

TABLE III
EFFECT OF PRESSURE

| T (°C) | P (kPa) | MEA inlet (kg mole/h) | $NH_3$ inlet (kg mole/h) | Product (kg mole/h) | EDA in Product (kg mole/h) | $NH_3$ excess (kg mole/h) | Yield | DETA in Product (kg mole/h) |
|---|---|---|---|---|---|---|---|---|
| 150 | 2000 | 4000 | 10000 | 14000 | 3472.000 | 6263.600 | 0.868 | 263.200 |
| 150 | 3000 | 4000 | 10000 | 14000 | 3613.400 | 6193.600 | 0.903 | 193.200 |
| 150 | 4000 | 4000 | 10000 | 14000 | 3693.200 | 6153.000 | 0.923 | 154.000 |
| 150 | 5000 | 4000 | 10000 | 14000 | 3743.600 | 6127.800 | 0.936 | 127.400 |
| 150 | 6000 | 4000 | 10000 | 14000 | 3777.200 | 6111.000 | 0.944 | 110.600 |

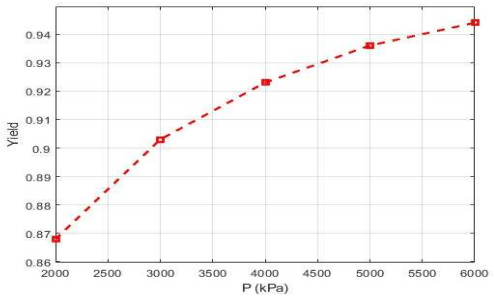


Fig. 6 Yield vs Pressure at T=150 C

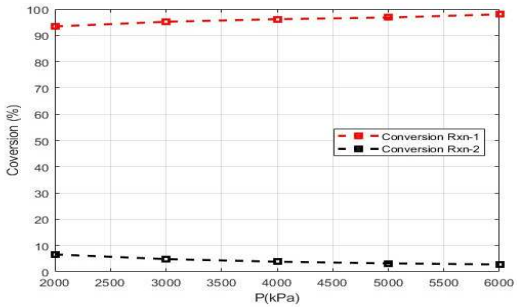


Fig. 7 Conversion vs Pressure at T=150 C

### D. Selectivity and Byproduct Formation

Selectivity towards EDA is a crucial performance measure in the catalytic process. The formation of DETA, a byproduct, competes with the desired EDA production. The simulation data shows that optimizing temperature and pressure, combined with careful catalyst management, can suppress the secondary reaction that leads to DETA formation. The optimal conditions of 150°C, 6000 kPa, and the correct catalyst loading achieved the highest selectivity, minimizing DETA to negligible levels. At the identified optimal conditions (150°C, 6000 kPa, and optimal catalyst loading), the selectivity towards EDA was maximized, with DETA formation kept to a minimum (Figs. 8 and 9). 7his indicates that careful control of operating parameters is essential for achieving high selectivity in the industrial production of EDA.

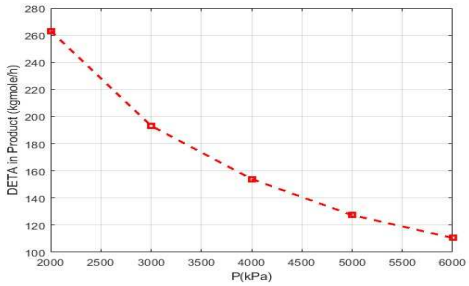


Fig. 8 DETA in Product vs P at 150 C

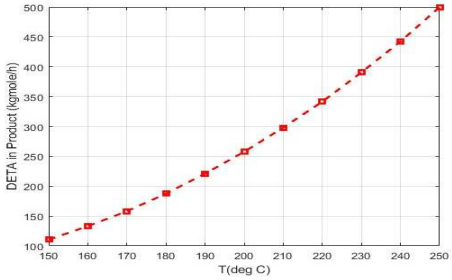


Fig. 9 DETA in Product vs T at 6000 kPa

### E. $NH_3$ to MEA Ratio

The ratio of NH3 to MEA also plays a critical role in optimizing reactor performance. The simulation results showed that the EDA yield improved as the NH3 to MEA ratio increased, stabilizing at a 1:14 ratio. Ratios beyond this point did not significantly enhance the yield, as the conversion of MEA approached completion (Table 4 and Fig. 10). These findings underline the importance of managing inlet ratios to optimize the overall reaction efficiency.

TABLE IV
$NH_3$ TO MEA RATIO

| Ratio | MEA inlet (kg mole/h) | NH3 inlet (kg mole/h) | Product (kg mole/h) | EDA in Product (kg mole/h) | NH3 excess (kg mole/h) | Yield | DETA in Product (kgmole/h) |
|---|---|---|---|---|---|---|---|
| 2 | 4000 | 8000 | 12000 | 3772.800 | 4113.600 | 0.943 | 114.000 |
| 3 | 4000 | 12000 | 16000 | 3784.000 | 8108.800 | 0.946 | 108.800 |
| 4 | 4000 | 16000 | 20000 | 3794.000 | 12102.000 | 0.949 | 102.000 |
| 5 | 4000 | 20000 | 24000 | 3804.000 | 16099.200 | 0.951 | 98.400 |
| 6 | 4000 | 24000 | 28000 | 3808.000 | 20095.600 | 0.952 | 95.200 |
| 7 | 4000 | 28000 | 32000 | 3814.400 | 24092.800 | 0.954 | 92.800 |
| 8 | 4000 | 32000 | 36000 | 3819.600 | 28090.800 | 0.955 | 90.000 |
| 9 | 4000 | 36000 | 40000 | 3824.000 | 32088.000 | 0.956 | 88.000 |
| 10 | 4000 | 40000 | 44000 | 3823.600 | 36088.800 | 0.956 | 88.000 |
| 11 | 4000 | 44000 | 48000 | 3830.400 | 40084.800 | 0.958 | 86.400 |
| 12 | 4000 | 48000 | 52000 | 3832.400 | 44085.600 | 0.958 | 83.200 |
| 13 | 4000 | 52000 | 56000 | 3830.400 | 48081.600 | 0.958 | 84.000 |
| 14 | 4000 | 56000 | 60000 | 3834.000 | 52080.000 | 0.959 | 84.000 |

### F. Performance Achieved in This Research

The simulation results demonstrate that the highest yield of ethylenediamine (EDA), 94.4%, was achieved at optimal operating conditions: a temperature of 150°C, pressure of 6000 kPa, and an *ammonia*-to-*monoethanolamine* ($NH_3$:MEA) molar ratio of 14:1. These conditions also minimized the formation of the primary byproduct, diethylenetriamine (DETA), to negligible levels (<5%). The results indicate that careful control of temperature, pressure, and feed ratios is critical for enhancing selectivity and efficiency in EDA production.

### G. Performance Achieved in This Research

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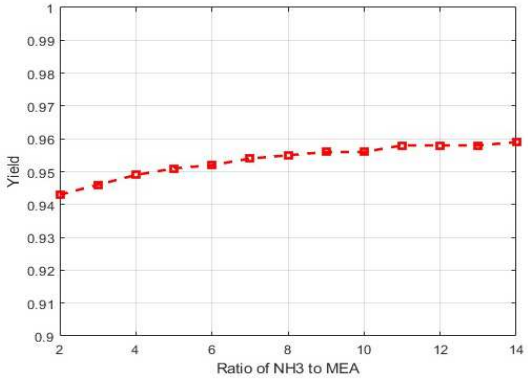


Fig. 10 Plot of Yield vs NH3 to MEA Ratio

### *H. Comparison with Previous Studies*

The performance metrics obtained in this study are compared to findings from previous research (Table 5) to highlight the improvements and advancements made:

TABLE V
COMPARISON WITH PREVIOUS STUDIES

| **Parameter** | **Current study** | [21] | **Key Differences** |
|---|---|---|---|
| EDA Yield (%) | 94.4 | 66.4 | Higher yield achieved due to optimal $NH_3$:MEA ratio, temperature, and pressure conditions. |
| Optimal Pressure (kPa) | 6000 | 8000 | Lower pressure improved equilibrium, aligning with Le Chatelier's principle. |
| Optimal Temperature (°C) | 150 | 170 | Lower temperature favored selectivity toward EDA over DETA. |
| $NH_3$:MEA Ratio | 14:1 | 10:1 | Demonstrates the benefit of a higher $NH_3$ feed ratio in reducing byproduct formation. |

### *I. Implications for Industrial Scale-Up*

The simulation findings have several implications for industrial-scale EDA production. Identifying optimal reactor conditions not only enhances yield but also reduces byproduct formation, leading to a more sustainable and cost-effective process. The ability to fine-tune operating parameters using tools like Aspen HYSYS allows industries to minimize waste and improve overall process efficiency, aligning with the growing focus on sustainable chemical manufacturing.

### *J. Limitation and Future Work*

While the simulation provided valuable insights, the accuracy of the model depends on the assumptions made, such as the reaction kinetics and thermodynamic data used. Future work should focus on experimental validation to ensure that the optimized conditions translate effectively to industrial applications. Further exploration into alternative catalysts and reactor configurations could improve EDA production efficiency.

## IV. CONCLUSION

This study provides a comprehensive investigation into optimizing ethylenediamine (EDA) production through the catalytic reaction of monoethanolamine (MEA) and ammonia in a heterogeneous plug-flow reactor (PFR). Utilizing Aspen HYSYS as a simulation tool, the research systematically evaluated key operational parameters, including temperature, pressure, and the ammonia-to-MEA molar ratio, to identify conditions that maximize yield while minimizing byproduct formation.

The findings demonstrate that the optimal conditions—150°C, 6000 kPa, and an ammonia-to-MEA ratio of 14:1—resulted in a maximum EDA yield of 94.4%. These conditions effectively minimize the formation of the byproduct diethylenetriamine (DETA), achieving high selectivity and efficiency. The study highlights the synergistic impact of operational parameter control and catalyst performance on process outcomes, advancing the understanding of heterogeneous catalytic processes for EDA synthesis.

Aspen HYSYS proved instrumental in simulating complex reaction systems and optimizing reactor performance, showcasing its potential as a critical industrial process design and control tool. The insights gained are pivotal for guiding future efforts to scale up EDA production, improve reactor configurations, and explore alternative catalytic systems to enhance sustainability.

Future research should focus on experimental validation of the optimized conditions, developing advanced catalyst formulations, and applying real-time monitoring systems to further refine the production process. By addressing both operational efficiency and environmental impact, this work supports the broader objective of promoting sustainable practices in the chemical manufacturing sector.

## ACKNOWLEDGMENT

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