Effect of Operating Temperature on Cyclohexane Recovery by Chiller in Solution Phase Polymerization

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Abstract— Cyclohexane, a critical solvent in solution-phase polyethylene polymerization, is often lost due to inefficient recovery in industrial processes. This study investigates the impact of chiller operating temperature on cyclohexane recovery efficiency in an existing petrochemical plant using Aspen HYSYS. It explores the influence of chiller operating temperature on the recovery of cyclohexane, a critical solvent in the solution phase polymerization process for polyethylene production. Using Aspen HYSYS, a simulation was conducted to analyze an existing solvent recovery system and propose modifications by incorporating an additional chiller. The results demonstrate that lower chiller temperatures significantly enhance cyclohexane recovery yields, with a recovery rate increasing from 83.5% to 89.0% as temperatures decrease from 75°C to 50°C. This improvement is attributed to enhanced condensation of vaporized cyclohexane at lower temperatures. However, lower temperatures increased chiller duty and required larger heat exchangers, this improvement comes with increased chiller duty and higher capital investment. Economic analysis indicates a total investment of approximately $746,900.735, a payback period of approximately 1.57 years for the modified system, highlighting its viability despite high initial costs. The findings highlight the critical role of temperature optimization in balancing recovery efficiency and operational costs, offering insights for improving solvent recovery in petrochemical plants.

Keywords — *Cyclohexane, Solvent Recovery; Chiller; Operating Temperature; Aspen HYSYS; Polyethylene; Solution Phase Polymerization; Cyclohexane Recovery; Solvent Recycling; Polyethylene Production; Chiller Optimization; Energy Efficiency; Petrochemical Economics.*

1. Introduction

Cyclohexane (C_6H_{12}), a cycloalkane is a vital solvent in the solution phase polymerization process for producing polyethylene, including high-density polyethylene (HDPE), low-density polyethylene (LDPE), and linear low-density polyethylene (LLDPE). Despite its importance, solvent recovery remains a significant challenge in petrochemical plants, with current systems recovering only about 83% of cyclohexane, leading to increased production costs (Aspen Tech et al., 2012). The exothermic nature of the polymerization process accelerates solvent vaporization, further complicating recovery efforts (Chanda et al., 2013). This study aims to enhance cyclohexane recovery by simulating an existing process using Aspen HYSYS and modifying it with an additional chiller to determine the effect of operating temperature on recovery efficiency.

The petrochemical industry faces both economic and environmental pressures to optimize solvent recovery. Cyclohexane is costly, and its importation significantly increases production expenses (McNaught et al., 1996). Additionally, solvent losses contribute to environmental concerns, necessitating efficient recovery systems that align with safety and sustainability standards (Hamley et al., 2004). This study aims to enhance cyclohexane recovery by modifying an existing plant's solvent recovery unit through the addition of a chiller and analyzing the effect of operating temperature on recovery efficiency using Aspen HYSYS simulation software.

The objectives include analyzing the current recovery process, ascertaining the optimum solvent recovery rate with a new chiller, evaluating the impact of temperature on recovery, and assessing the economic benefits of the proposed modification. The research addresses the high cost of solvent loss, the energy intensive nature of recovery, and the need for sustainable and cost-effective solutions in polyethylene production.

2. Material and Methods

2.1 Materials and Simulation Setup

The simulation was conducted using Aspen HYSYS, selected for its robust thermodynamic models and comprehensive database for chemical engineering simulations (Aspen Tech et al., 2012), employing the Non-Random Two-Liquid (NRTL) model to calculate phase equilibria, accounting for the non-ideal behavior of the liquid phase in the recovery process The process involved vapor streams from the Intermediate Pressure Separator (IPS) and Low Pressure Separators (LPS 1 and LPS 2), primarily containing cyclohexane, butene-1, butene-2, unconverted ethylene, ketones, and water (Warn hoff et al.,

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1996). The simulation basis involved specifying the fluid package, component list, and process conditions, including temperature, pressure, flow rate, and composition. Cyclohexane served as the primary solvent, while other components represented typical constituents in the polymerization process, key equipment included splitters, heat exchangers, and chillers, with design specifications.

2.2 Simulation Procedure

Equipment: The simulation was conducted using Aspen HYSYS software on a computer system. Key equipment modeled included:

- *Splitters:* Used to separate cyclohexane from other components in the stream.
- *Heat Exchangers:* Employed as condensers to cool and condense vaporized cyclohexane.
- *Chillers:* Added to enhance cooling and improve recovery efficiency.

The simulation followed these steps:

a Define the simulation basis
- Start a new case in Aspen HYSYS.
- Select the NRTL fluid package from the fluid package tab.
- Specify components: cyclohexane, butene-1, butene-2, ethylene, ketones, and water.

b Building the Simulation Environment:
- Add material streams and unit operations (splitters, heat exchangers, chillers) from the object palette.
- Configure streams with inlet conditions (e.g., IPS stream as the solution adsorber).
- Connect unit operations, specifying inlet and outlet streams (e.g., IPS to LPS 1 and LPS 2).

c Inputting Process Variables:
- Vary chiller temperatures between 50°C and 75°C.
- Specify pressure, flowrate, and composition based on plant data (Campbell et al., 2011).

d Optimizing Recovery:
- Adjust heat exchanger and chiller temperatures to maximize cyclohexane recovery.
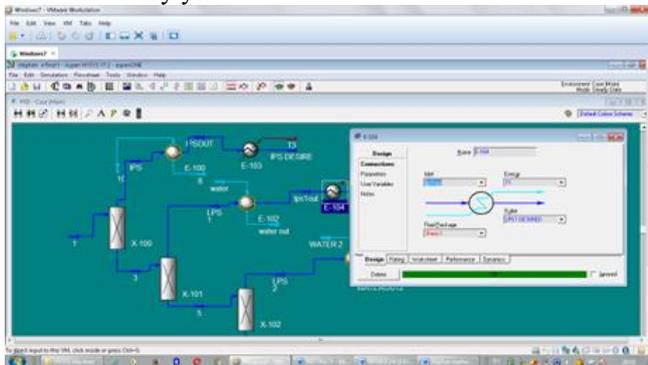- Monitor the effect of temperature on chiller duty and recovery yield.
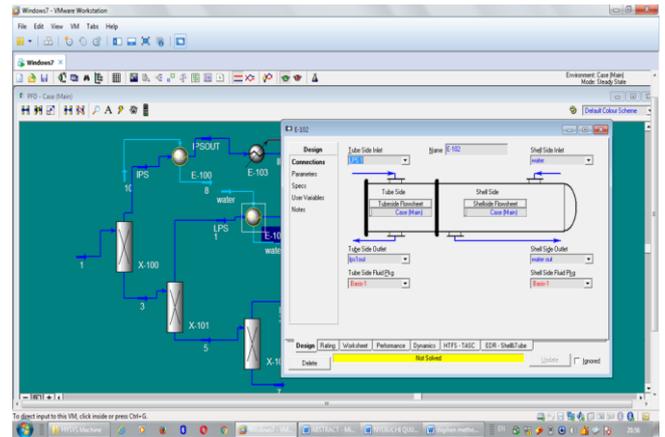

Fig.1: Window showing chiller

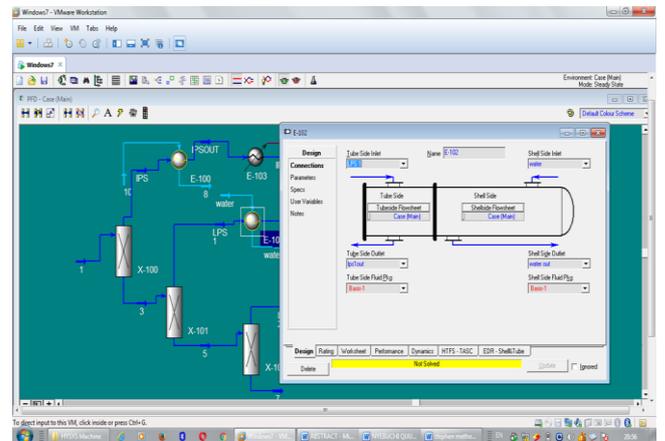**Fig.2: Window showing heat exchanger**

Fig. 3: Window showing simulated plant

3. Experimental Design

The experimental design focused on simulating the existing solvent recovery process and modifying it by incorporating a chiller to enhance cyclohexane recovery. The process flow included:

IPS Stream: The initial vapor stream from the Intermediate Pressure Separator, containing cyclohexane and other components.

LPS Streams: Two low-pressure separators (LPS 1 and LPS 2) further processed the IPS outlet to separate cyclohexane.

Chillers: Added to the IPS and LPS streams to provide additional cooling, enhancing condensation (Campbell et al., 2011). The simulation varied the chiller operating temperature across five cases (50°C, 60°C, 65°C, 70°C, 75°C) to evaluate its impact on recovery yield and chiller duty. The NRTL model was employed to model phase equilibria, as described by the equation:

$$\ln(\gamma_i) = \frac{\sum_{j=1}^{n} x_j \tau_{ji} G_{ji}}{\sum_{k=1}^{n} x_k G_{ki}} + \sum_{j=1}^{n} \frac{x_j G_{ij}}{\sum_{k=1}^{n} x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_{m=1}^{n} x_m \tau_{mj} G_{mj}}{\sum_{k=1}^{n} x_k G_{kj}} \right)$$

NTRL Equation (www. users.rowan.edu)

where $G_{ij} = exp(-\alpha_{ij}\tau_{ij})$, and τ_{ij} incorporates temperature-dependent interaction parameters (Chremos et al., 2014). The heat balance was modeled using:

$Q = UA \cdot LMTD \cdot F_t = Mhot\ (Hin - Hout)hot - Qloss = Mcold\ (Hout - Hin)cold - Qleak$

Where:
- U is the overall heat transfer coefficient,
- A is the heat transfer area,
- *LMTD is the log mean temperature difference, and*
- F_t is the correction factor (Campbell et al., 2011).

4. Statistical Analysis and Correlation

The simulation data were analyzed to establish relationships between chiller temperature, recovery yield, and chiller duty. Key variables included:

- Independent Variable: Chiller operating temperature (50℃ to 75℃).
- Dependent Variables: Cyclohexane recovery yield (%), chiller duty (kW), and heat exchanger area (m²).

A linear regression analysis was conducted to quantify the relationship between temperature and chiller duty, revealing a strong negative correlation ($R^2 > 0.95$), indicating that lower temperatures significantly increase the energy required for cooling (Aspen Tech et al., 2012). Similarly, recovery yield exhibited a negative correlation with temperature, as lower temperatures enhanced condensation, increasing the liquid cyclohexane recovered (Warnhoff et al., 1996). The correlation between temperature and recovery yield was also strong ($R^2 > 0.90$), confirming the effectiveness of temperature reduction in improving recovery. Economic metrics, including total investment (TI) and payback period (PBP), were analyzed to assess cost-effectiveness. The payback period was calculated as:

$$PBP = \frac{Total\ Investment\ (TI)}{Annual\ Savings}$$

Where, annual savings were derived from reduced cyclohexane losses (Campbell et al., 2011). The analysis showed a significant reduction in PBP as recovery yield increased, particularly between 83.5% and 86.2%, highlighting the economic benefits of enhanced recovery.

5. Result and Discussion

5.1 Chiller Duty and Temperature

The simulation results for three product streams (IPS Desired, LPS 1 Desired, LPS 2 Desired) are summarized in Table 1. As the chiller temperature decreased from 75℃ to 50℃, the chiller duty increased linearly, consistent with the heat transfer equation (Campbell et al., 2011). For the IPS Desired stream, the duty increased from 500 kW at 75℃ to

750 kW at 50℃, reflecting the higher energy required to achieve lower temperatures.

Table 1: Chiller Duty at Various Temperatures for IPS Desired Stream

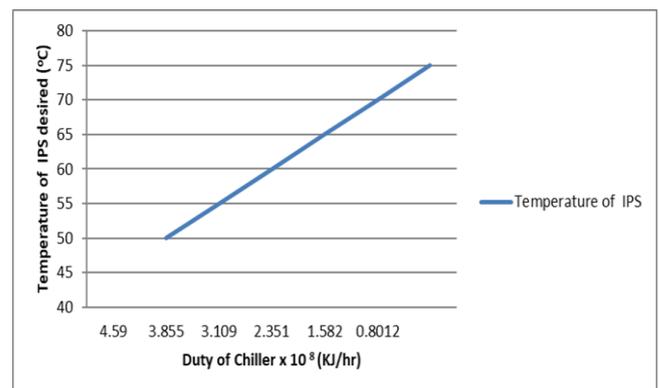| Temperature (℃)	Chiller Duty (kW)
75	500
70	550
65	600
60	675
50	750

Fig.4: Effect of Temperature on Chiller Duty

Figure 5 and 6 illustrates this linear relationship, emphasizing the trade-off between cooling efficiency and energy consumption.
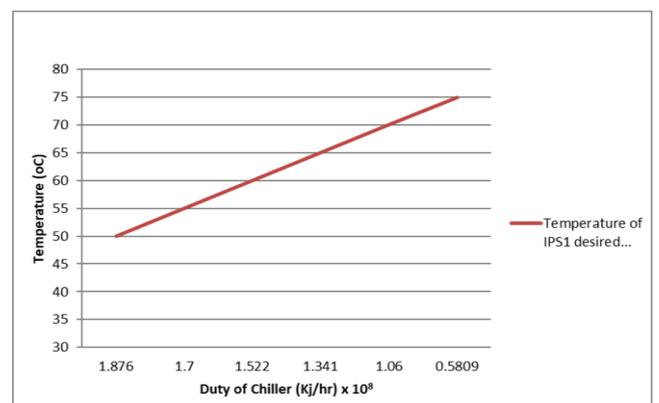

Fig.5: Effect of Temperature on Chiller Duty
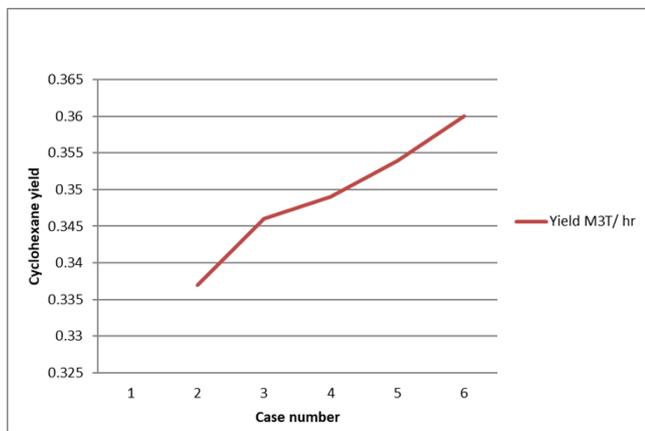
5.2 Cyclohexane Recovery Yield

The recovery yield of cyclohexane increased with decreasing chiller temperature, as shown in Table 2. At 75℃, the recovery yield was 83.5%, while at 50℃, it reached 89.0%. This improvement is attributed to enhanced

condensation of vaporized cyclohexane at lower temperatures, reducing losses to the vapor phase (Warnhoff et al., 1996).

Table 2: Cyclohexane Recovery Yield at Various Temperatures

Temperature (°C)	Recovery Yield (%)
75	83.5
70	83.5
65	86.2
60	87.5
50	89.0

Figure 7 illustrates the increase in recovery yield with decreasing temperature, confirming the effectiveness of the chiller modification (Chanda et al., 2013).
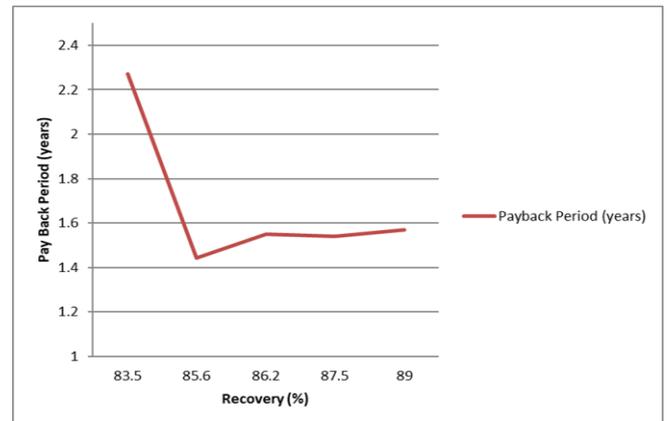

Fig.6: Graph of Cyclohexane yield for Cast

Fig. 7: Cyclohexane Recovery Unit (Indorama Manual, 1998)

5.3 Economic Analysis

The economic analysis evaluated the trade-off between increased recovery yield and capital investment, as summarized in Table 3. As recovery yield increased, the heat exchanger area and chiller size grew, raising the total investment. However, the payback period decreased significantly, from 2.28 years at 83.5% to 1.57 years at 89.0%, due to reduced cyclohexane losses.

Table 3: Economic Analysis of Recovery Yields

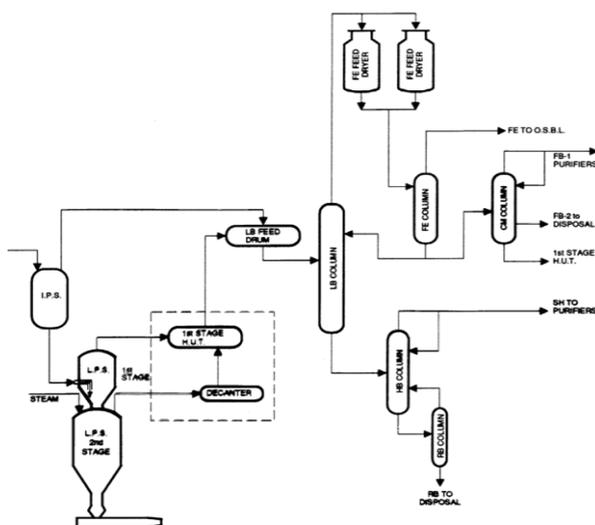| Case	Recovery Yield (%)	Total Investment ($)	Payback Period (Years)
1	83.5	338,035.381	2.28
2	83.5	394,347.36	1.44
3	86.2	479,639.08	1.55
4	87.5	596,292.38	1.54
5	89.0	746,900.735	1.57

Fig. 8: Graph of Payback Period on Recovery Yield

Figure 9 illustrates the reduction in payback period with increasing recovery yield, highlighting the economic benefits of the modified system.

5.4 Discussion

The results confirm that chiller operating temperature is a pivotal parameter in cyclohexane recovery. Lower temperatures enhance condensation, increasing the liquid cyclohexane recovered but necessitating higher chiller duties and larger heat exchangers (Warnhoff et al., 1996). This aligns with the heat transfer equation, where increased temperature differences drive higher heat transfer rates (Campbell et al., 2011). The addition of a chiller significantly improved recovery yields, addressing the limitations of the existing process, which relied on three heat exchangers with limited efficiency.

The economic analysis underscores the trade-off between capital investment and operational savings. While the modified system requires a substantial investment of $746,900, the short payback period of 1.57 years justifies its implementation. This finding is consistent with industry trends toward optimizing solvent recovery to reduce costs and environmental impact (Hamley et al., 2004). The use of Aspen HYSYS provided a robust platform for modeling complex phase equilibria, enabling precise predictions of recovery performance under varying conditions (Chremos et al., 2014).

The study's limitations include the steady-state simulation mode, which may not capture transient behaviors, and the reliance on data from a single petrochemical plant (Campbell et al., 2011). Future research should explore dynamic simulations and additional parameters, such as pressure and flow rate, to further optimize the process (Hadjichristidis et al., 2003).

6. Discussion

Operating temperature plays a pivotal role in the solvent recovery process. Lower temperatures significantly enhance cyclohexane recovery but also increase operational energy demand. This study demonstrates that reducing chiller operating temperatures significantly enhances cyclohexane recovery in solution phase polymerization, achieving yields up to 89.0% at 50℃. The addition of a chiller to the existing recovery system addresses the limitations of the current setup, which recovers only 83.5% of cyclohexane. The modified system is economically viable, with a total investment of $746,900 and a payback period of 1.57 years. The findings underscore the importance of optimizing operating conditions to balance recovery efficiency and cost, offering a practical solution for petrochemical plants. Continued research into dynamic simulations and other process parameters will further enhance recovery efficiency and sustainability.

These findings emphasize the importance of optimizing operating conditions to balance recovery efficiency and cost, offering a practical solution for petrochemical plants. Continued research into dynamic simulations and other process parameters will further enhance recovery efficiency and sustainability (Hamley et al., 1998).

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