

Improvement of Cyclohexane Recovery Unit in a Polyethylene Plant: Process Optimization and Economic Evaluation

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Abstract — This study presents a comprehensive approach to improving Cyclohexane recovery in a polyethylene production plant through process optimization and equipment modification. The current solvent recovery system, which utilizes three shell-and-tube heat exchangers in series, achieves only 83% recovery efficiency, leading to significant economic losses and environmental concerns. Cyclohexane is an indispensable solvent in the solution phase polymerization process critical for the manufacturing of diverse polyethylene products, including high-density (HDPE), low-density (LDPE), and linear low-density polyethylene (LLDPE). Despite its pivotal role, industrial operations frequently encounter substantial challenges in achieving comprehensive solvent recovery, leading to considerable economic penalties and an escalation in overall production costs. This comprehensive study undertakes an in-depth investigation into advanced methodologies aimed at enhancing cyclohexane recovery within an established polyethylene production facility. The research employs sophisticated process simulation techniques, specifically utilizing Aspen HYSYS, to model and analyze proposed modifications to the existing solvent recovery unit. A central focus is placed on assessing the impact of integrating a new condenser, referred to as a "chiller," and meticulously examining how variations in operating temperatures influence both solvent recovery efficiency and the energy duty required by the chiller.

The empirical findings from the simulation rigorously demonstrate a pronounced inverse correlation between decreasing operating temperature and an increase in the volume of cyclohexane recovered. Concomitantly, this enhanced recovery at lower temperatures is directly linked to a significant rise in the energy duty demanded by the chiller. While the initial capital investment associated with the installation of these chillers is substantial, estimated at approximately \$746,900.735, the projected economic analysis reveals a highly favorable and short payback period of approximately 1.57 years. This rapid return on investment strongly underscores the economic viability and strategic benefits of implementing such process enhancements. Ultimately, this study furnishes a detailed blueprint of simulated optimal operating conditions for superior cyclohexane recovery, thereby offering invaluable practical insights and a robust framework for the design, development, and optimized operation of future and existing polyethylene manufacturing facilities.

Keywords — Cyclohexane Recovery; Process Optimization; Polyethylene Production; Solvent Recycling; Aspen HYSYS Simulation; Heat Integration.

1. Introduction

1.1 The Crucial Role of Polyethylene and Cyclohexane

In the contemporary industrial landscape, polymer products are ubiquitous, permeating nearly every facet of daily life, from packaging to construction materials. Among these, polyethylene stands out as one of the most widely produced and utilized polymers globally. Its versatility, attributed to varying densities and molecular structures, makes it suitable for an extensive range of applications. The manufacturing of polyethylene, particularly through solution phase polymerization, relies heavily on the use of specialized solvents to facilitate the reaction and subsequent processing steps. Cyclohexane (C₆H₁₂), a cyclic alkane, is a primary solvent employed in this critical industrial process. Its molecular structure and chemical properties make it an

ideal medium for the synthesis of High-Density Polyethylene (HDPE), Low-Density Polyethylene (LDPE), and Linear Low-Density Polyethylene (LLDPE), among others. Beyond its role in polyethylene, cyclohexane is also a significant precursor in nylon generation and is commercially produced through the hydrogenation of benzene. Notably, the demand for cyclohexane contributes approximately 11.4% to the global demand for benzene, highlighting its strategic importance in the petrochemical sector (Warnhoff, 1996).

1.2 The Challenge of Solvent Recovery in Petrochemical Plants

Despite the indispensable role of cyclohexane, modern polyethylene production processes are consistently confronted with a persistent and economically significant challenge: the inefficient recovery of the solvent post-

polymerization. In the specific petrochemical plant that serves as the basis for this study, the current solvent recovery unit manages to recover only about 83% of the cyclohexane in circulation. This recovery is achieved through a system comprising three separate shell and tube heat exchangers, which function as condensers. While these units perform their intended purpose to some extent, the suboptimal recovery rate translates directly into substantial financial burdens. The continuous loss of a valuable and often imported solvent necessitates frequent replenishment, thereby inflating operational expenditures and diminishing overall profitability.

The problem statement for this research is thus clearly defined: to address the prevalent issue of inadequate solvent (cyclohexane) recovery in existing polyethylene process plants. The imperative is to devise and evaluate solutions that can significantly increase the solvent recovery rate, leading to a substantial reduction in production costs and enhancing the plant's economic competitiveness. The aim is not merely to recover the solvent but to achieve maximum achievable profit under optimal operating conditions, while strictly adhering to environmental and safety regulations.

2. Aim and Objectives

The overarching aim of this study is to enhance the efficiency of the solvent (cyclohexane) recovery process within an existing polyethylene plant. This will be achieved through a rigorous simulation and analysis of the current process, followed by the modeling of targeted modifications. The study is structured around the following specific objectives:

- To conduct a comprehensive analysis of the existing cyclohexane recovery process, identifying bottlenecks and areas for improvement.
- To ascertain the optimal rate of solvent recovery that can be achieved through the strategic addition of a new condenser, specifically a chiller, to the existing recovery unit.
- To meticulously determine the precise effect of varying operating temperatures on the efficiency of solvent recovery by the chiller, thereby identifying ideal temperature profiles.
- To perform a detailed economic analysis, quantifying the additional volume of cyclohexane recovered as a direct consequence of the proposed modification and calculating the cumulative cost savings realized from reduced solvent losses.

2.1 Justification of Study

The justification for undertaking this research is multifaceted and compelling. The continuous losses of cyclohexane in existing polyethylene plants directly lead to

increased production costs, impacting the economic viability and competitiveness of these operations. By proffering a lasting and effective solution to these losses, this study contributes directly to enhancing the profitability and sustainability of the petrochemical industry. Furthermore, optimizing solvent recovery aligns with broader industrial goals of resource efficiency, waste minimization, and environmental responsibility. The insights gained from this simulation-based study will provide actionable intelligence for process engineers and plant managers seeking to upgrade their existing facilities or design new, more efficient polyethylene production units.

3. Survey of the Literature

3.1 Polymerization Processes and Inherent Solvent Recovery Challenges

Polymerization, the process by which monomer molecules react chemically to form polymer chains, is foundational to the plastics industry. Many industrial polymerization processes, particularly those involving heterogeneous catalysts, rely on the use of a solvent. This solvent acts as a medium to ensure intimate contact between the catalyst particles and the monomers, facilitating the reaction. The resulting effluent stream from such processes is typically a complex mixture containing the desired polymer dissolved in the solvent, unreacted monomers, and residual catalyst particles.

The subsequent separation of the solvent from this intricate mixture is not merely a technical step but a crucial economic and environmental imperative. Achieving a high-purity finished polymer product, free from catalyst residues and solvent traces, is a primary goal. More significantly, from an economic standpoint, the solvents employed in these processes are often expensive, and their loss represents a direct financial drain. Therefore, the efficient recovery and recycling of the solvent are paramount for cost-effectiveness and overall process sustainability (Warnhoff, 1996).

However, the separation of solvents from polymer slurries is fraught with engineering complexities. A common challenge arises from the nature of the polymer itself, some polymer components may remain dissolved in the solvent, while others might be dispersed within it. Traditional solvent recovery methods, such as simple evaporation, often lead to an increase in the viscosity of the remaining polymer-solvent mixture as the solvent is removed. This increasing viscosity can severely impede further vaporization or evaporation of the hydrocarbon solvent, making complete solvent removal from the molten or concentrated solution exceedingly difficult. For high-molecular-weight polymers, the solution's viscosity can escalate very rapidly with increasing polymer concentration,

creating a "viscous consistency" that makes product recovery extremely challenging. This necessitates the development and implementation of advanced, highly efficient separation techniques and robust solvent recovery units capable of handling such complex fluid dynamics.

3.2 Role of Cyclohexane and Industrial Polymerization Methods

Cyclohexane, with its specific molecular structure (C₆H₁₂) and non-polar characteristics, has been identified as a highly suitable solvent for solution phase polymerization processes, particularly in the context of polyethylene production. Its properties allow for effective dissolution of monomers and polymers, as well as efficient heat transfer within the reactor. Warnhoff (1996) explores the history and properties of cyclohexane in detail, emphasizing its suitability as a solvent. The reduction of aromatic compounds, such as benzene to cyclohexane, has been a subject of research, with early methods exploring the use of phosphonium iodide (Baeyer, 1870; Zhang et al., 2008). Industrially, polymerization reactions are conducted using various techniques, each with its own advantages and disadvantages concerning heat management, product form, and solvent handling (Michael, 2005). These methods include:

- **Bulk Polymerization:** Carried out without any solvent or dispersant. While simple in formation, the exothermic nature of many chain-growth polymerizations can lead to rapid heat generation and control difficulties, often requiring efficient cooling systems (Chanda, 2013).
- **Solution Polymerization:** The method directly relevant to this study. Here, monomers are dissolved in a solvent. This approach offers excellent heat dispersion and easier mixing compared to bulk polymerization due to lower viscosity. However, careful selection of the solvent is critical to prevent unwanted chain-transfer reactions with the growing polymer chains. The challenge often lies in the subsequent removal of the solvent from the viscous polymer product, especially if the polymer is not intended for commercial use in solution form.
- **Suspension Polymerization:** Monomers are dispersed in an immiscible liquid (typically water) via vigorous stirring and stabilizers. Heat is efficiently dispersed by the aqueous medium, yielding polymers in granular or bead form.
- **Emulsion Polymerization:** Involves the formation of a stable emulsion of monomer in water using emulsifying agents. A water-soluble free-radical initiator initiates polymerization within monomer droplets (micelles). This method allows for very high molecular weights and effective heat dissipation but can be complex in formulation and purification.
- **Gas-Phase Polymerization:** Utilized for gaseous monomers, where monomers diffuse to growing

polymer chains within a reaction vessel, yielding a granular solid polymer (Prince, 1995).

Understanding these different methods underscores the specific challenges and opportunities associated with solvent recovery in solution polymerization, emphasizing why targeted improvements to cyclohexane units are essential (McNaught & Wilkinson, 1996).

3.3 Computer Simulation in Chemical Engineering: The Aspen HYSYS Advantage

In the modern chemical process industry, computer simulation has transitioned from a theoretical concept to an indispensable tool for every stage of a plant's lifecycle, from conceptual design to operational optimization. These powerful simulation software packages employ sophisticated models that incorporate approximations and assumptions to accurately represent real-world chemical processes. They provide engineers with an unparalleled ability to determine process variables, predict material and energy balances, and estimate other critical properties of the system without the need for costly and time-consuming physical experiments.

Among the leading simulation software, Aspen HYSYS stands out as a robust and widely utilized platform, particularly for the simulation of process plants and refineries (Aspen Tech, 2012). Its distinguishing features include:

- **Extensive Database:** A comprehensive library of pure component data and phase equilibrium information, with the flexibility to incorporate user-defined components.
- **Reliable Thermodynamic Models:** A wide array of rigorous thermodynamic models, crucial for accurate predictions of phase behavior and energy requirements.
- **Rigorous Equipment Models:** Detailed models for various unit operations (e.g., heat exchangers, columns, reactors, compressors), enabling precise sizing, performance evaluation, and optimization.
- **User-Friendly Interface:** An intuitive graphical interface that enhances usability and streamlines workflows, facilitating rapid model construction and analysis.
- **Integrated Tools:** Features for energy optimization (e.g., pinch analysis), preliminary cost estimation, and detailed exchanger modeling, allowing for holistic process evaluation.
- **Open Architecture:** Compatibility with third-party tools and CAPE-OPEN standards, enabling seamless integration of external models and property packages.

The application of Aspen HYSYS in this study is justified by its ability to facilitate the rapid evaluation of various design alternatives and operating conditions. It

allows engineers to create interactive models and sensitivity analyses, which are critical for identifying optimal process parameters. This capability significantly reduces engineering costs, accelerates the design cycle, and empowers better decision-making throughout the plant's operational life.

One of the key thermodynamic models frequently employed in Aspen HYSYS and relevant to this study is the Non-Random Two-Liquid (NRTL) model. The NRTL model is an activity coefficient model used to correlate the activity coefficients of compounds with their mole fractions in the liquid phase. It is particularly valuable for calculating phase equilibria in non-ideal liquid mixtures, such as those encountered in solvent recovery processes. The model is predicated on the hypothesis that the local concentration of molecules around a central molecule deviates from the bulk concentration. This deviation arises from differences in the interaction energy between the central molecule and molecules of its own kind versus molecules of other kinds, introducing a "non-randomness" at the molecular level. This theoretical foundation allows NRTL to accurately predict the phase behavior of complex mixtures, which is essential for designing efficient separation units like condensers and chillers.

4. Methodology: Process Simulation and Modeling Approach

The methodology revolves around a comprehensive simulation-based approach to investigate and improve cyclohexane recovery within a polyethylene production facility. This involved a meticulous process of modeling an existing solvent recovery unit and then implementing and analyzing proposed modifications, specifically the integration of new cooling equipment.

4.1 Materials and Equipment (Simulated)

The simulation necessitated a precise definition of the chemical components involved and the unit operations to be modeled.

4.1.1 Process Materials

The primary feed stream under investigation was the vapor stream emanating from the Intermediate Pressure Separator (IPS) and Low Pressure Separators (LPS). This stream, rich in components that need separation, comprised:

- *Cyclohexane (SH)*: The target solvent for recovery.
- *Butene-1 (FB-1)* and *Butene-2 (FB-2)*: Other hydrocarbon components.
- *Unconverted Ethylene (FE)*: Unreacted monomer.
- *Ketones and Water*: Impurities or by-products. Accurate characterization of these components and their

thermodynamic properties was critical for reliable simulation results.

4.1.2 Simulated Equipment

The Aspen HYSYS software environment allowed for the virtual construction of the solvent recovery unit using standard chemical engineering unit operations. These included:

- *Splitters*: Used to divide process streams into two or more outlet streams, enabling the separation of different phases or components based on defined criteria.
- *Heat Exchangers (Condensers)*: Modeled as shell and tube heat exchangers, these units are crucial for cooling vapor streams to promote condensation and solvent recovery. Their design parameters, such as heat transfer area and heat transfer coefficients, were defined within the simulation.
- *Chillers*: Representing advanced cooling technology, chillers were introduced as the key modification to enhance condensation and recovery efficiency, especially at lower temperatures. The entire computational work, including model building, parameter variation, and data analysis, was performed using a dedicated computer system equipped with the Aspen HYSYS software (Aspen Tech, 2012).

4.2 Algorithm for Simulation

A systematic and iterative algorithm guided the simulation process, ensuring a logical progression from initial setup to optimized product recovery. The algorithm can be conceptualized as follows:

- *Feed Stream Input*: Define the inlet feed stream characteristics, including its temperature, pressure, total molar flow rate, and detailed molar or mass compositions of all components. This step establishes the baseline conditions of the existing process.
- *Introduction of Splitters*: Integrate splitter unit operations into the flowsheet. These splitters represent physical separation points where different phases (e.g., vapor and liquid) or components are directed to subsequent units. For instance, an initial splitter would handle the stream from the Intermediate Pressure Separator (IPS), directing a vapor-rich stream to the recovery section.
- *Integration of Chillers*: Introduce the new chiller units at strategic points within the solvent recovery loop. These chillers are designed to provide sub-ambient cooling, forcing the condensation of cyclohexane that might otherwise remain in the vapor phase.
- *Integration of Heat Exchangers (Condensers)*: Model the existing heat exchangers (condensers) in series or parallel, connecting them appropriately to the chillers and other separation units. These units work in

conjunction with the chillers to cool the cyclohexane-rich stream and facilitate condensation.

- *Temperature Variation for Optimization:* Crucially, the operating temperature of the heat exchangers (and by extension, the chillers) is systematically varied across a defined range. This sensitivity analysis is performed to identify the optimal temperature conditions that maximize the recovery of the desired product (cyclohexane).
- *Desired Product Analysis:* The properties of the outlet streams, particularly the recovered liquid cyclohexane, are meticulously analyzed at each varied temperature setting. This includes evaluating the purity, flow rate, and overall recovery percentage of cyclohexane.

This algorithmic approach allowed for a systematic exploration of the process behavior under different conditions and the identification of optimal operating points.

4.3 HYSYS Simulation Procedure

The practical implementation of the simulation in Aspen HYSYS involved a structured, multi-step procedure:

4.3.1 Defining the Simulation Basis

The foundational step in any HYSYS simulation is defining the "simulation basis," which includes the thermodynamic models and components.

- *Start a New Case:* Initiated a new simulation project within Aspen HYSYS.
- *Specify Fluid Package:* Navigated to the "Fluid Package" tab in the simulation basis manager. For this study, the NRTL (Non-Random Two-Liquid) Fluid Package was selected. The NRTL model was chosen for its ability to accurately predict the vapor-liquid equilibrium (VLE) of the non-ideal mixtures encountered in cyclohexane recovery, which include polar components like water and ketones alongside hydrocarbons.
- *Select Components:* Added all relevant chemical components to the fluid package from the HYSYS component library. This included Cyclohexane (SH), Butene-1 (FB-1), Butene-2 (FB-2), Ethylene (FE), Ketones, and Water. Accurate property data for these components are crucial for the simulation's validity.

4.3.2 Entering the Simulation Environment (Recreation Condition)

Once the basis was defined, the simulation moved to the "simulation environment" where the process flowsheet was constructed by adding and connecting material streams and unit operations (Aspen Tech, 2012).

4.3.2.1 Material Streams Definition

- Streams were added from the object palette and dropped onto the simulation environment.
- Each stream was then double-clicked to input its specific conditions:
 - *Temperature (°C):* Initial temperature of the stream.
 - *Pressure (kPa):* Initial pressure of the stream.
 - *Molar Flow (kgmole/hr):* The total flow rate of the stream.
 - *Composition (Mole Fraction):* The individual mole fractions of each component (Cyclohexane, Butene-1, Ethylene, etc.).
- This detailed definition was applied to all inlet streams, particularly the vapor feeds from the IPS and LPS units.

4.3.2.2 Adding Splitters

- Splitter units were selected from the object palette and placed on the flowsheet.
- Connections were established an "Inlet Stream" (e.g., from an IPS or LPS) and multiple "Outlet Streams" (e.g., liquid cyclohexane rich stream and a vapor stream containing lighter components).
- The function of the splitter was to facilitate the separation of the desired cyclohexane from other components in the stream, often based on phase separation or component distribution ratios.

4.3.2.3 Adding Heat Exchangers (Condensers)

- Heat exchanger units were added to the simulation environment.
- Connections were made for the "Hot Side Inlet/Outlet" and "Cold Side Inlet/Outlet" streams. In the context of condensers, the hot side would be the process fluid (cyclohexane-rich vapor) and the cold side would be the cooling utility.
- The primary function of these condensers was to provide cooling to condense the vaporized cyclohexane.

4.3.2.4 Adding Chillers

- Chiller units were introduced as the key enhancement. Similar to heat exchangers, they were connected with an inlet process stream and an outlet stream, alongside a utility stream (energy stream).
- For example, a chiller was connected to the "IPS OUT" stream to produce the "IPS DESIRED" stream, representing the recovered cyclohexane.
- The chillers were designed to provide aggressive cooling to further condense cyclohexane that might have escaped the initial condensers, thereby boosting overall recovery.

The entire process involved an iterative approach of adding, connecting, and configuring these unit operations. Parameters within each unit (e.g., heat transfer coefficients for exchangers, target temperatures for chillers) were adjusted as part of the optimization process. This meticulous simulation setup allowed for a detailed analysis of flow, energy, and material balances throughout the modified recovery unit.

4.4 Modeling Equations

The accuracy of process simulation hinges on the underlying mathematical models that govern physical and chemical phenomena. This study primarily relied on two key modeling frameworks.

4.5 Non-Random Two-Liquid (NRTL) Model

As previously mentioned, the NRTL equation is a crucial activity coefficient model frequently employed in chemical engineering to calculate phase equilibria, particularly for non-ideal liquid mixtures. It correlates the activity coefficients of a compound i (γ_i) with its mole fractions in the liquid phase concerned (x_i).

The NRTL model is based on the premise that the local concentration around a molecule differs from the bulk concentration due to variations in interaction energies between molecular species. This energy difference introduces a "non-randomness" at the local molecular level, making it effective for mixtures exhibiting significant deviations from ideal behavior.

The general form of the NRTL equation for the activity coefficient of component i in a multi-component mixture is:

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

Where:

- γ_i : Activity coefficient of component i .
- x_i : Mole fraction of component i .
- τ_{ij} , τ_{ji} : Non-randomness parameters representing the interaction energy between components i and j .
- $G_{ij} = \exp(-\alpha_{ij}\tau_{ij})$ and $G_{ji} = \exp(-\alpha_{ji}\tau_{ji})$: Local composition parameters.
- α_{ij} : Non-randomness factor, typically a constant, with $\alpha_{ij} = \alpha_{ji}$.

These parameters (τ_{ij} , α_{ij}) are typically temperature-dependent and are determined from experimental vapor-liquid equilibrium data. Aspen HYSYS contains an extensive database for these parameters, allowing for robust VLE calculations essential for accurate separation predictions in the condensers and chillers.

4.6 Heat Balance Equation

The heat balance equation is fundamental for analyzing the energy transfer within the heat exchangers and chillers. It allows for the calculation of the heat duty (Q) required or removed by these units. For a heat exchanger or condenser, the rate of heat transfer is proportional to the overall heat transfer coefficient, the heat transfer area, and the temperature driving force.

The simplified heat balance equation employed is:

$$Q = UA(LMTD)F_i = M_{hot}(H_{in} - H_{out})_{hot} - Q_{loss} = M_{cold}(H_{out} - H_{in})_{cold} - Q_{leak}$$

Where:

- Q : Total heat transfer rate (e.g., chiller duty, in KJ/hr).
- U : Overall heat transfer coefficient ($W/m^2 \cdot K$ or similar units), which accounts for the resistances to heat transfer across the fluid films and the heat exchanger wall.
- A : Total heat transfer surface area (m^2) available for heat exchange.
- $LMTD$: Log Mean Temperature Difference ($^{\circ}C$ or K), the effective average temperature difference between the hot and cold fluids across the heat exchanger.
- F_i : LMTD correction factor, applied for complex flow arrangements (e.g., multi-pass shell and tube exchangers) to adjust for non-ideal temperature profiles.
- M_{hot} : Mass flow rate of the hot fluid (process stream).
- $(H_{in} - H_{out})_{hot}$: Enthalpy change of the hot fluid across the exchanger.
- M_{cold} : Mass flow rate of the cold fluid (cooling utility or process stream being heated).
- $(H_{out} - H_{in})_{cold}$: Enthalpy change of the cold fluid across the exchanger.
- Q_{loss} , Q_{leak} : Terms representing heat losses to the surroundings or heat leakages into the system, which are generally minimized in efficient designs.

This equation was critically applied to evaluate the energy requirements (chiller duty) as the operating temperature of the desired product streams was varied. The direct relationship between increased duty and decreased temperature, as observed in the results, directly conforms to this heat transfer principle.

5. Results and Discussion

The simulation results provided profound insights into the intricate relationship between operating parameters, particularly temperature, and the efficiency of cyclohexane recovery, alongside the associated economic implications. The analysis focused on three distinct product streams: IPS

desired, LPS 1 desired, and LPS 2 desired, representing the recovered cyclohexane from different stages of the separation process.

5.1 Effect of Operating Temperature on Chiller Duty and Cyclohexane Yield

The simulations consistently revealed a strong, linear dependence of the chiller's energy duty on the operating temperature of the desired product stream. Specifically, a decrease in the target operating temperature for the recovered cyclohexane streams invariably led to a significant increase in the energy duty required from the chiller. This observation is in perfect concordance with the fundamental principles of heat transfer and thermodynamics, achieving lower temperatures necessitates the removal of a greater amount of heat, which, in turn, demands more energy input to the refrigeration cycle of the chiller.

For instance, detailed data for the IPS desired stream (Table 1) showed that as the temperature was progressively reduced within the range of 50–75°C, the corresponding chiller duty consistently escalated. A similar and equally pronounced trend was observed for the LPS 1 desired stream (Table 2), further reinforcing the direct correlation between lower temperatures and increased energy consumption by the cooling units. The simulation also highlighted an optimal operating point for the IPS2 desired stream, which was achieved specifically at 77°C (Table 3). Any deviation from this temperature, either higher or lower, resulted in a suboptimal recovery of this particular stream, indicating a narrow operational window for maximizing its yield.

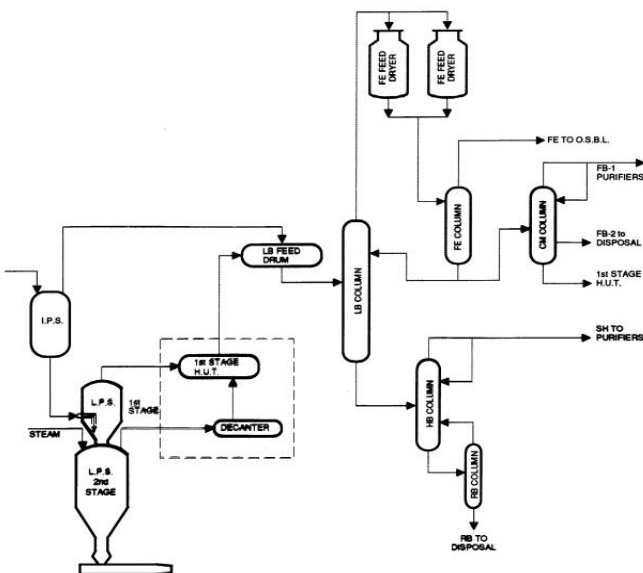


Fig. 1: Cyclohexane Recovery Unit (Indorama Manual, 1998)

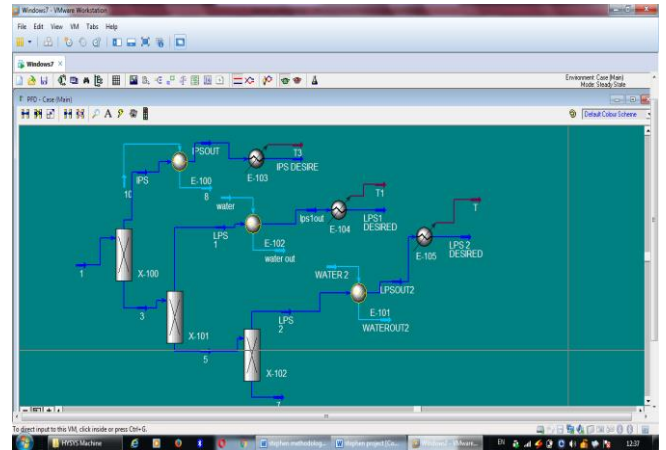


Fig. 2: Window showing simulated plant

Table 1. Effect of stream temperature (IPS desired) change

Temperature of IPS desired (°C)	Chiller		
	Change in Pressure (Kpa)	Temperature change (°C)	Duty of Chiller(Kj/hr)
50	196.1	-30	4.590 x 10 ⁸
55	196.1	-25	3.855 x 10 ⁸
60	196.1	-20	3.109 x 10 ⁸
65	196.1	-15	2.351 x 10 ⁸
70	196.1	-10	1.582 x 10 ⁸
75	196.1	-5	8.012 x 10 ⁷

Table 2: Effect of stream temperature (IPS 1 desired) change

Temperature of IPS1 desired (°C)	Chiller		
	Change in Pressure (Kpa)	Temperature change (°C)	Duty of Chiller (Kj/hr.)
50	49.03	-35	1.876 x 10 ⁸
55	49.03	-30	1.700 x 10 ⁸
60	49.03	-25	1.522 x 10 ⁸
65	49.03	-20	1.341 x 10 ⁸
70	49.03	-15	1.060 x 10 ⁸
75	49.03	-10	5.809 x 10 ⁷

Table 3. Effect of stream temperature (IPS 2 desired) change

Temperature of IPS 2 desired (°C)	Chiller		
	Change in Pressure (Kpa)	Temperature change (°C)	Duty of Chiller (Kj/hr)
75	-	-	-
77	51.12	-1	126

Crucially, the relationship between operating temperature and the overall cyclohexane yield presented an inverse proportionality, the yield of recovered cyclohexane substantially increases as the operating temperature decreases (Table 4). This phenomenon is directly attributable to the thermodynamic principle of condensation. At lower temperatures, the vapor pressure of cyclohexane is significantly reduced, facilitating more extensive condensation of cyclohexane from the vapor phase into the liquid phase. This leads to a greater volume of liquid solvent being recovered. This finding underscores the critical importance of precise and controlled temperature management within the chiller units for achieving maximal solvent recovery efficiency. Optimizing this balance between energy expenditure (chiller duty) and recovery yield is a key engineering challenge.

Table 4. Effect of stream temperature on Recovered Cyclohexane yield

Case number	Operating Condition Temperature (°C)			Yield M ³ T/ hr	Recovery %
	IPS	LPS1	LPS2		
1	75	75	77	0.337	83.5
2	70	70	77	0.346	85.6
3	65	65	77	0.349	86.2
4	60	60	77	0.354	87.5
5	55	55	77	0.360	89

5.2 Economic Analysis: Cost-Benefit Assessment of Enhanced Recovery

The economic analysis conducted as part of this study provided a compelling argument for the financial viability of integrating chillers into the cyclohexane recovery unit, despite the initial capital investment required. This analysis is crucial for justifying the proposed modifications from a business perspective. Calculations for the economic analysis were based on methods described in Coulson and Richardson's "Chemical Engineering Plant Design."

- **Installation Cost:** The upfront capital expenditure for installing the new chillers in a cyclohexane plant was found to be substantial. For Case 5 (89% recovery), the Total Investment Required (TIR) was estimated at approximately \$746,900.735 (Table 5) This figure encompasses the cost of the chiller units themselves, associated piping, insulation, electrical connections, and installation labor, with calculations adjusted for the 2017 cost index based on a 2007 baseline. Such a significant investment typically necessitates a robust financial justification.
- **Payback Period:** Despite the considerable initial outlay, the simulated economic model projected a remarkably short payback period. For Case 1 (83.5% recovery), the payback period was 2.28 years, while for Case 5 (89% recovery), it was approximately 1.57 years (Table 5). The payback period is a critical financial metric that

indicates the time required for the cumulative cash inflows from a project (in this case, savings from reduced solvent losses) to offset the initial investment. A short payback period suggests a rapid return on investment, making the project highly attractive from a financial standpoint. This rapid recoupment of costs is primarily driven by the substantial savings realized from the increased recovery and subsequent reduced purchase of expensive, imported cyclohexane.

- **Recovery vs. Investment:** The analysis meticulously explored the relationship between the cyclohexane recovery ratio and the Total Investment (TI) required, as well as its impact on the payback period. It was observed that as the recovery ratio increases, the Total Investment (TI) also tends to increase. This is a logical consequence, as achieving higher recovery rates often necessitates larger heat exchange surface areas (for more efficient cooling and condensation) and potentially more sophisticated or larger chiller units, which inherently contribute to higher equipment and installation costs.

However, a crucial and insightful observation was the inverse relationship between the recovery rate and the payback period (PBP): as the recovery rate increases, the payback period generally decreases (Table 5). This signifies that the economic benefits of increased solvent recovery (due to reduced operational costs) outweigh the incremental increase in capital investment. The study presented different "cases" for varying recovery percentages.

Table 5. Summary of Economic Analysis of Simulated plant

Case number	Recovery %	Total Investment Required	Cumulative Cash flow	Payback Period (years)
1	83.5	\$338,035.381	\$4,457,538.00	2.28
2	85.6	\$394,347.36	\$8,201,869.92	1.44
3	86.2	\$479,639.08	\$9,271,679.04	1.55
4	87.5	\$596,292.38	\$11,589,598.80	1.54
5	89	\$746,900.735	\$14,264,121.60	1.57

While the payback period for Case 3 and Case 4 showed a slight increase or negligible difference compared to Case 2 despite higher recovery, the overall trend from 83.5% to 89% recovery indicates a significant reduction in payback period. This suggests an optimal point beyond which the diminishing returns on payback period reduction might warrant a trade-off with increased capital outlay, but the general direction of profitability is clear. The consistent reduction in the payback period with increased yield of recovered cyclohexane strongly supports the economic justification for the proposed modifications.

Thus, the economic analysis unequivocally supports the financial feasibility and significant benefits of modifying the existing cyclohexane recovery unit with the integration of chillers. The rapid recoupment of the initial investment through operational savings highlights a clear pathway for industries to achieve both enhanced process efficiency and improved financial performance.

6. Conclusion

Drawing upon the comprehensive simulation results and detailed economic analysis, the following definitive conclusions can be established regarding the strategic improvement of the cyclohexane unit for solvent recovery within a polyethylene plant:

- *Profound Impact of Operating Temperature:* The operating temperature of the chiller exerts a profound and direct influence on the volume of Cyclohexane recovered. It has been conclusively demonstrated that even a slight reduction in temperature significantly impacts the energy duty required by the chiller, while simultaneously leading to a substantial increase in the volume of cyclohexane condensed and recovered. This highlights temperature as a critical control variable for maximizing solvent capture.
- *Economic Viability of Chiller Installation:* Despite the initially capital-intensive nature of installing chillers in a cyclohexane plant, estimated at approximately \$746,900.735, the projected economic returns are highly favorable. The remarkably short simulated payback period of approximately 1.57 years unequivocally demonstrates the strong economic viability and attractive return on investment associated with this process modification. The long-term operational savings stemming from reduced solvent loss quickly offset the initial outlay.
- *Direct and Inverse Correlations:* A clear and consistent direct correlation exists between the required energy duty of the chiller and the magnitude of the temperature change achieved. Conversely, an inverse relationship is firmly established between the operating temperature and the cyclohexane recovery yield: lower temperatures directly translate to higher percentages of solvent recovered. This dual relationship underscores the critical balance between energy consumption and recovery efficiency that must be optimized.

In summary, the integration of chillers represents a technically sound and economically attractive solution for significantly enhancing cyclohexane recovery in polyethylene plants, leading to both operational efficiency and substantial cost savings.

References

- [1] Aspen Technology. (2012). Aspen HYSYS User Guide. Burlington, MA: Aspen Technology Inc.
- [2] Baeyer, A. (1870). Ueber die Reduction aromatischer Kohlenwasserstoffe durch Jodphosphonium. *Annalen der Chemie und Pharmacie*, 155, 266–281.
- [3] Bates, F. S., & Fredrickson, G. H. (2014). Block Copolymer Thermodynamics: Theory and Experiment. *Annual Review of Physical Chemistry*, 41, 525–557.
- [4] Campbell, M. L. (2011). Cyclohexane. *Ullmann's Encyclopedia of Industrial Chemistry*.
- [5] Chanda, M. (2013). *Introduction to Polymer Science and Chemistry* (2nd ed.). CRC Press.
- [6] Chremos, A., Nikoubashman, A., & Panagiotopoulos, A. (2014). Flory-Huggins parameter, from binary mixtures of Lennard-Jones particles to block copolymer melts. *Journal of Chemical Physics*.
- [7] Eisenbach, C. D., & Heinemann, T. (1995). Thermoplastic graft copolymer elastomers with chain-folding or bifurcated side chains. *Macromolecular Chemistry and Physics*, 196(8), 2669–2686.
- [8] Zhang, F. F., van Rijnman, T., Kim, J. S., & Cheng, A. (2008). *On Present Methods of Hydrogenation of Aromatic Compounds, 1945 to Present Day*. Lunds Tekniska Högskola.
- [9] Gazit, O., Khalfin, R., Cohen, Y., & Tannenbaum, R. (2009). Self-assembled diblock copolymer "nanoreactors" as catalysts for metal nanoparticle synthesis. *Journal of Physical Chemistry C*, 113, 576–583.
- [10] Hadjichristidis, N., Pispas, S., & Floudas, G. (2003). *Block Copolymers: Synthetic Strategies, Physical Properties, and Applications*. Wiley.
- [11] Hamley, I. W. (1998). *The Physics of Block Copolymers*. Oxford University Press.
- [12] Hamley, I. W. (2004). *Developments in Block Copolymer Science and Technology*. Wiley.
- [13] Mayer, J., Urban, S., Habrylo, S., Holderna, K., Natkaniec, I., Würflinger, A., & Zajac, W. (1991). Neutron Scattering Studies of C6H12 and C6D12 Cyclohexane under High Pressure. *Physica Status Solidi (b)*, 166(2), 381.
- [14] McNaught, A. D., & Wilkinson, A. (1996). *Glossary of basic terms in polymer science (IUPAC Recommendations 1996)*. *Pure and Applied Chemistry*, 68, 2287–2311.
- [15] Prince, D. M. (1995). Temperature Calibration of Differential Scanning Calorimeters. *Journal of Thermal Analysis*, 45(6), 1285–1296.
- [16] Warnhoff, E. W. (1996). The Curiously Intertwined Histories of Benzene and Cyclohexane. *Journal of Chemical Education*, 73(6), 494.
- [17] Musser, M. T. (2005). Cyclohexanol and Cyclohexanone. *Ullmann's Encyclopedia of Industrial Chemistry*. Wiley-VCH.