Journal of Vocational Studies on Applied Research, 7 (2), 2025, 59–64

Contents lists available at JVSAR website

Journal of Vocational Studies on Applied Research

Journal homepage: https://ejournal2.undip.ac.id/index.php/jvsar

Research Article

Energy Efficiency Improvement Through Pinch Analysis of Gas Phase Chlorination Process of Propylene

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Abstract

Dependence on imports of raw materials such as allyl chloride amid the rapid development of the national chemical industry is the background for optimizing energy efficiency in the preliminary design of this 15,000 ton/year capacity plant. Given that the production process involves an exothermic gas phase chlorination reaction at extreme temperatures (510 K), the use of Pinch Technology is crucial to minimizing energy consumption. This study utilizes HINT software to identify heat and cold flows, set the most favorable ΔTmin temperature threshold, and formulate a Composite Curve to map the potential for heat integration in the system. The research shows that through the identification of pinch points; the Maximum Energy Recovery (MER) target can be achieved by integrating waste heat from the reactor outlet stream to independently heat the feed before it enters the furnace unit. The implementation of this optimized heat exchanger network has been proven to significantly reduce the use of external utilities, such as Dowtherm A and cooling water, which ultimately lowers the plant's total annual costs. Overall, the application of pinch technology-based heat management strategies is a fundamental step in strengthening the economic value and operational sustainability of allyl chloride production.

Article history:
Received: 29th December 2025
Revised: 31st December 2025
Accepted: 31st December 2025
Available online: 31st December 2025
Published: 31st December 2025

Keywords:
Allyl Chloride
Pinch Technology
Maximum Energy Recovery
Heat Exchanger Network

Permalink/DOI: http://doi.org/10.14710/jvsar.v7i2.30768

1. Introduction

Pinch technology represents a thermodynamic approach to heat integration, aimed at establishing the minimum requirements for heating and cooling utilities by pinpointing pinch points and developing composite curves. Originating in the late 1970s amid the global energy crisis, this method offers a structured framework for uncovering inefficiencies and constraints in industrial heat recovery systems (Linnhoff & Hindmarsh, 1983). Central to pinch analysis is the principle that heat exchange across the pinch point should be minimized to prevent unnecessary escalation in external utility demands (March, 1998).

In the initial design phase of an allyl chloride facility, pinch technology assumes significant relevance owing to the intensely exothermic gas-phase chlorination reaction, which proceeds at high temperatures around 510 °C. The substantial thermal output from the reactor effluent presents opportunities for internal heat reclamation, potentially serving to warm feed streams and diminish reliance on external heating sources. By merging pinch analysis with Heat Exchanger Network (HEN) synthesis, it becomes possible to concurrently enhance energy efficiency and optimize investments in heat transfer apparatus, including furnaces, coolers, and condensers, thus lowering the overall annual operational expenses (Hall et al., 1990).

Pinch analysis facilitates the recognition of thermodynamic limitations in chemical operations through the formulation of composite curves that delineate the system's energy supply and demand profiles (Kemp, 2006). A pivotal parameter in this analysis is the minimum temperature difference (ΔTmin), which influences the balance between energy conservation and heat exchanger surface area. Lower ΔTmin values typically enhance energy recuperation but necessitate greater surface areas and associated capital outlays, while higher values curtail equipment expenditures at the cost of elevated utility usage

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(Gilani & Morosuk, 2025).

Despite its extensive adoption across chemical sectors, there remains a need for deeper exploration of heat integration in the preliminary design of an allyl chloride plant with an annual output of 15,000 tons, especially to curtail the use of Dowtherm A and cooling water. Advancements in pinch technology have broadened its scope from mere energy targeting to holistic process integration, encompassing operational adaptability and economic refinement (Rani et al., 2023). Investigations into analogous chlorination processes have demonstrated energy savings of up to 30%, accompanied by payback periods of 2–3 years through robust heat integration measures (Philia et al., 2020).

Consequently, this research endeavors to assess the prospects for heat reclamation from reactor effluent streams, ascertain the optimal ΔTmin, and formulate an energy-efficient and cost-effective Heat Exchanger Network to bolster the sustainability of allyl chloride manufacturing (Ravagnani et al., 2005; Widayat et al., 2022). Such an approach not only addresses immediate efficiency gains but also contributes to broader evaluations of thermodynamic constraints, potentially revealing trade-offs that could inform more resilient process designs in volatile energy markets.

2. Methods

2.1 Description of the Allyl Chloride

The production of allyl chloride in this design relies on a gas-phase chlorination reaction involving propylene and chlorine. The process encompasses several stages: vaporization of feeds, preheating, high-temperature reaction within a multitube fixed-bed reactor, rapid quenching, and product separation via distillation. The chlorination reaction follows a free-radical mechanism at temperatures ranging from 420 to 510 °C, yielding allyl chloride as the primary product alongside hydrogen chloride as a by-product (Li et al., 2021).

The reactor's multitube fixed-bed design ensures efficient heat dissipation, thereby sustaining near-isothermal conditions amid the exothermic nature of the reaction. The reactor effluent, comprising unreacted propylene, allyl chloride, hydrogen chloride, and minor by-products, emerges at approximately 510 Kand serves as a substantial source of recoverable thermal energy in the process (Seider et al., 2017). This hot stream necessitates cooling to appropriate temperatures before separation, while the propylene and chlorine feed streams demand heating from ambient levels to the reaction temperature.

Drawing from the temperature variations in the Heater, Vaporizer, and Cooler units depicted in the Process Flow Diagram (PFD), process streams are categorized as hot or cold in line with pinch analysis methodologies. Streams that require cooling are designated as hot streams, and those needing heating are classified as cold streams (March, 1998). The pronounced temperature disparity between the reactor effluent and the feed streams underscores a significant opportunity for heat integration via pinch technology (Kemp, 2006). This approach warrants critical examination to optimize energy efficiency and minimize operational costs in the chlorination process.

2.2 Data Extraction

Data for heat integration analysis is derived from the outcomes of mass and heat balance computations in process design. Key parameters encompass mass flow rate, heat capacity (CP), inlet temperature (Tin), and outlet temperature (Tout), all of which are vital for ascertaining the thermal attributes of individual process streams (March, 1998). The extraction process prioritizes principal streams traversing heat exchanger equipment, such as heaters and coolers, to pinpoint avenues for energy conservation via internal heat reclamation. The precision and thoroughness of this extracted data are paramount, as they underpin the ensuing pinch analysis and Heat Exchanger Network (HEN) synthesis (Towler & Sinnott, 2022).

Subsequent to data extraction, streams are categorized as either hot, necessitating cooling, or cold, requiring heating. Within the allyl chloride manufacturing process, hot streams predominantly comprise the reactor effluent at roughly 510 Kand various product streams that demand cooling before separation stages. Cold streams encompass propylene and chlorine feedstocks that must be elevated from storage temperatures to reaction levels, alongside reboiler loads in distillation operations. The thermal attributes of each stream, notably the heat capacity flow rate (CP), dictate the gradient of streams on temperature-enthalpy plots and profoundly shape the

Table 1. Process stream data for pinch analysis.

Stream	Stream Type	Mass Flow (kg/h)	Cp Mean (kW/K)	Tin (K)	Tout (K)	ΔT (K)
6	Hot	1893.939	1.589214116	318.15	303.15	15
7	Hot	109.634	1.236670254	364.15	303.15	61
10	Hot	3587.374	1.236670254	309.15	303.15	6
15	Cold	1789.38	1.236670254	303.15	329.15	26
1	Cold	2886.192	1.236670254	303.15	609.15	306
4	Cold	4821.633	1.236670254	783.15	323.15	460

viability and scope of heat integration across the system (Kemp, 2006; Seider et al., 2017). This characterization underscores the necessity for meticulous data handling to maximize thermodynamic efficiencies, potentially mitigating operational costs while enhancing process resilience in energy-intensive sectors. In this study, the extracted data is shown in Table 1.

2.3 *Pinch Analysis*

In the refining sector, pinch technology is extensively acknowledged as a robust approach for enhancing energy efficiency and mitigating environmental consequences. A case study applying pinch analysis to a contemporary crude distillation unit achieving 93% energy efficiency revealed that opportunities for additional energy conservation were constrained, underscoring the necessity of establishing pragmatic energy objectives in process integration investigations.

Pinch analysis serves to ascertain the minimal heating and cooling utility demands of a process. A pivotal element in this methodology is the minimum temperature difference (ΔTmin), which represents the narrowest permissible temperature interval between hot and cold streams, balancing heat recovery against the costs of heat exchanger infrastructure (Hall et al., 1990). The primary phases of pinch analysis encompass the formulation of a Problem Table, the determination of the pinch point, and the development of Composite Curves to illustrate the system's energy dynamics (March et al., 1998).

The Problem Table approach entails the sequential transfer of heat across temperature intervals, incorporating the ΔTmin constraint, culminating in the identification of the pinch point at the interval devoid of net heat excess (Linnhoff & Hindmarsh, 1983). Composite Curves offer a visual depiction of the aggregated heat supply from hot streams and the aggregated heat requirement of cold streams plotted against temperature. The minimal vertical distance between these curves equates to ΔTmin, with their nearest intersection denoting the pinch temperature, which imposes thermodynamic limitations on heat exchanger network configuration (Kemp, 2006; Linnhoff & Ahmad, 1990).

Selecting an appropriate ΔTmin demands meticulous evaluation of the interplay between energy conservation and capital outlays. Lower ΔTmin values facilitate enhanced heat recuperation and diminished utility usage, yet they necessitate expanded heat transfer surfaces and elevated capital investments. Conversely, higher ΔTmin values curtail capital expenditures while elevating operational expenses. Economic optimization often involves minimizing the Total Annual Cost (TAC), encompassing annualized capital and operational expenditures (Gilani & Morosuk, 2025; Linnhoff & Ahmad, 1990). For elevated-temperature chemical processes, such as allyl chloride synthesis, optimal ΔTmin values generally range from 10 to 30 °C, contingent upon specific process attributes and economic factors (Kemp & Lim, 2019). This selection process merits rigorous scrutiny to align with broader sustainability goals in industrial operations.

3. Result And Discussion

3.1 *Heat Exchanger Network (HEN) Design*

The Heat Exchanger Network (HEN) configuration (Figure 1) was conceptualized by drawing directly from the layout of operational units in the Allyl Chloride plant's Process Flow Diagram (PFD) (Figure 2) and the hot and cold stream data, with the aim of maximizing internal heat recovery while preserving the fundamental process architecture (Towler & Sinnott, 2022). Given the reaction temperature in Reactor (R-01) of 510 K, substantial thermal potential exists for integration with propylene and chlorine feed streams that necessitate preheating prior to entry into Furnace (F-01). The design approach adheres to the pinch design method, wherein stream pairings are executed methodically above and below the pinch point to uphold thermodynamic viability and curtail utility demands (Linnhoff & Hindmarsh, 1983).

Heat load determinations for each stream pair, such as the coupling of the hot product effluent from the reactor with the cold feed flow, rely on the Tin, Tout, and CP flow data derived from the initial heat balance. The thermal duty for a specific heat exchanger is computed via Q = m × CP × ΔT, where m denotes the mass flow rate, CP the specific heat capacity, and ΔT the temperature differential (Seider et al., 2017). The projected heat exchanger surface area for pivotal components, including Cooler (E-01) and Condenser (CDP-01), is ascertained using A = Q/(U × ΔTLM), with U representing the overall heat transfer coefficient and ΔTLM the logarithmic mean temperature difference (Towler & Sinnott, 2022).

The quantity of heat exchangers within the network is established to meet minimum energy objectives aligned with pinch principles, yielding a configuration that minimizes external utility inputs such as cooling water and Dowtherm A. The minimum number of units can be approximated by Nmin = Nstreams - 1,

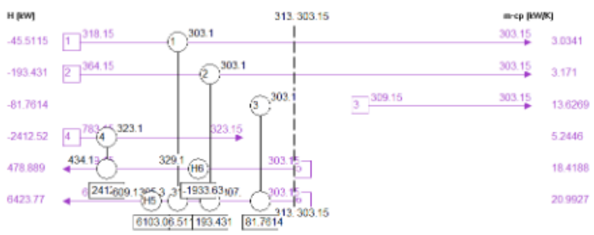

Figure 1. Heat Exchanger Network (HEN) Design.

though practical implementations may necessitate supplementary units to address process-specific requirements and operational factors (Linnhoff et al., 1994). Above the pinch point, cold streams undergo heating via hot streams or hot utilities, contingent on the heat capacity flow rate of hot streams equaling or surpassing that of cold streams (CP hot ≥ CP cold) to sustain thermodynamic integrity (Kemp, 2006). Below the pinch point, hot streams are cooled through cold streams or cold utilities, adhering to the inverse criterion (CP cold ≥ CP hot) to avert temperature inversions (March, 1998).

The incorporation of reactor effluent heat into feed preheating emerges as a pivotal element in this HEN design. Leveraging the sensible heat from the reactor outlet stream at 510 K to warm propylene and chlorine feeds can markedly diminish the thermal requirement from the furnace (Widayat et al., 2022). Such integration not only curtails Dowtherm A usage but also elevates overall process efficacy by reclaiming waste heat that might otherwise dissipate via cooling water. The design framework must incorporate pragmatic limitations, including pressure drop thresholds, equipment placement logistics, and operational adaptability to manage process disturbances or load variations (Ravagnani et al., 2005). This approach highlights the critical role of precise thermodynamic modelling in balancing energy recovery with system reliability, thereby informing more sustainable industrial practices amid escalating energy demands.

3.2 *Heat Integration Analysis*

Based on the simulation results using HINT software on the flow diagram in the document, optimal energy efficiency is achieved through the application of pinch technology that systematically integrates hot and cold flows. This analysis was conducted by identifying steam from the top of the Rectifying Column as a heat flow whose energy is transferred to heat the feed or reboiler in the Mash Column as a cold flow. Physicochemical parameter data, including temperature and heat flow rate, were processed using HINT software to produce a composite curve that determines the pinch point or minimum temperature limit. This point serves as a reference in designing a heat exchanger network, where energy requirements above the pinch point will be met by external utilities such as steam, while requirements below it will use cooling media. Figure 3 shows the PFD after pinch technology application.

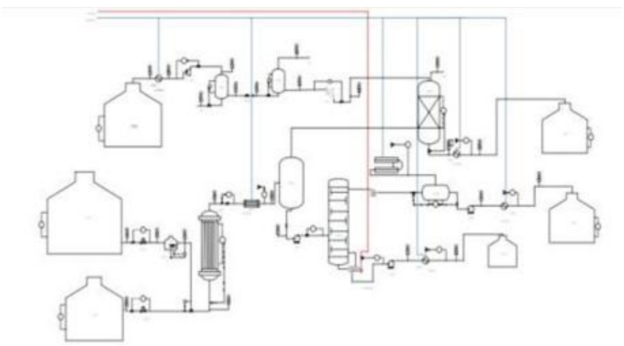

Figure 2. PFD before pinch technology application.

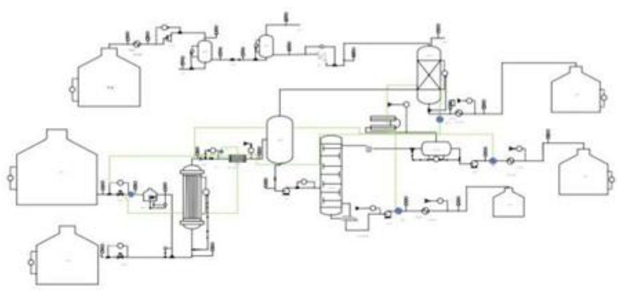

Figure 3. PFD after pinch technology application.

The application of heat integration through this HINT design facilitates the achievement of Maximum Energy Recovery (MER), which has been proven to significantly reduce steam consumption in reboilers and cooling water requirements in condensers. Modifications to the process flow, both in the Othmer configuration and the vacuum system, show that the pinch principle effectively reduces total operating costs by reusing waste heat in the system. This phenomenon reinforces the theory that setting a smaller ΔTmin value in the will increase energy savings potential, although it requires more investment in the heat transfer area of the heat exchanger (Riyanto et al., 2019). Overall, the use of pinch technology in the diagram confirms that integrated heat management is a key strategy in reducing total production costs.

Table 2 summarizes the comparison of heating and cooling utility demands before and after the implementation of pinch analysis with a minimum temperature difference of 10 K. Before heat integration was applied, the process depended solely on external utilities, leading to relatively high heating and cooling requirements of 8483.69 kW and 4457.06 kW, respectively. Following the application of pinch technology, both utility loads were substantially reduced, with the heating demand dropping to 4313.25 kW and the cooling demand to 143.81 kW. A total of 4169.44 kW of energy was successfully recovered and reused within the process, primarily for preheating cold streams by utilizing waste heat from hot streams. This outcome confirms that pinch analysis plays a significant role in improving energy efficiency by increasing internal heat utilization and reducing

Table 2. Comparison of energy requirements before and after pinch analysis (ΔTmin = 10K)

Condition	Heating Load (kW)	Cooling Load (kW)	Recovered Energy (kW)
Before pinch analysis	8483.69	4457.06	-
After pinch analysis	4313.25	143.81	4169.44

dependence on external heating and cooling utilities.

Figure 4 shows two main lines, namely the heat composite curve, which represents the energy availability of flows that require cooling (such as condenser steam), and the cold composite curve, which shows the energy requirements for flows that must be heated (such as mash feed). Visually, the temperature difference between the streams is indicated by the vertical distance, while the amount of energy exchanged is reflected by the horizontal distance between the two curves.

The point with the closest distance between these two curves is identified as the Pinch Point, which is the critical threshold in determining the energy efficiency of the system. The area where the two curves overlap horizontally represents the potential Maximum Energy Recovery (MER), which is heat that can be reused internally without requiring an external energy source. Conversely, the gap in the cold curve that exceeds the heat curve at the top indicates the need for additional energy from the heating utility (hot utility), while the gap in the heat curve at the bottom indicates the energy load that must be discharged through the cooling utility (cold utility).

4. Conclusion

Heat integration analysis using Pinch Technology with the help of HINT software in the preliminary design of an Allyl Chloride plant concluded that this method effectively optimizes energy efficiency through the systematic utilization of internal heat. Determining the pinch point plays a crucial role in setting the minimum temperature limit for separating the external heating utility (hot utility) above the pinch and the external cooling (cold utility) below the pinch. Through composite curve visualization, significant Maximum Energy Recovery (MER) potential was identified, whereby exothermic heat from the reactor outlet stream at 510 K could be diverted to independently heat the cold feed stream before it enters the furnace unit. The implementation of this integrated heat exchanger network (HEN) has been proven to reduce steam or Dowtherm A utility consumption in the reboiler and drastically reduce the cooling water load on the condenser compared to conventional designs. The simulation results confirm that selecting the appropriate ΔTmin value creates an optimal balance between operational cost savings and the investment value of the heat transfer area, thereby minimizing the factory's total annual costs. Overall, the application of pinch technology in this process flow diagram proves that integrated heat management is a fundamental strategy in improving the energy efficiency and economic value of Allyl Chloride and other chemical commodities.

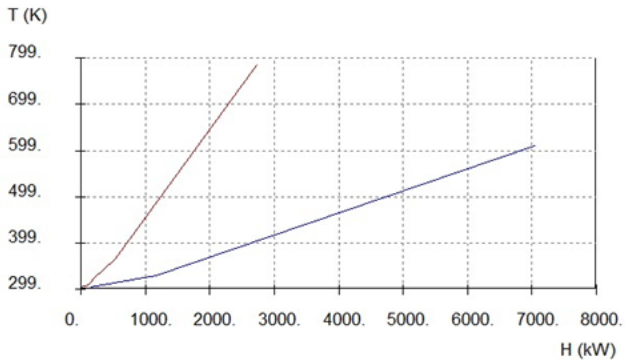

Figure 4. Composite curve.

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