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Hybrid Pinch-Analysis and MILP-Based Optimization for Energy and Water Recovery in a Bioethanol Plant

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The urgent need for sustainable and renewable energy has positioned bioethanol as a promising alternative to fossil fuels due to its biodegradability, reduced carbon footprint, and potential to utilize lignocellulosic biomass, yet conventional production processes remain highly energy- and water-intensive, threatening economic feasibility and environmental sustainability. This study presents a hybrid optimization methodology that integrates Pinch Analysis and Mixed Integer Linear Programming (MILP) to systematically enhance heat and water recovery in a lignocellulosic bioethanol plant. Pinch Analysis was first applied to identify thermodynamic efficiency targets, revealing potential energy savings of up to 38 % through strategic heat exchanger network design and water reuse opportunities, after which a MILP model was developed to determine cost-optimal hot–cold stream matches, exchanger placements, and water reuse configurations, ensuring feasibility while minimizing utility consumption and capital expenditures. Results demonstrated that the hybrid approach reduced hot and cold utility requirements by more than 40 % compared to baseline operations, while freshwater intake and wastewater discharge were lowered by approximately 30–35 %. Furthermore, integration of Life Cycle Assessment (LCA) confirmed that the optimized process achieved a 28 % reduction in greenhouse gas emissions, a 22 % decrease in cumulative energy demand, and a 30 % improvement in water footprint, with additional reductions in acidification and eutrophication impacts, thereby validating the environmental benefits of the optimization framework. Overall, the combined thermodynamic and mathematical programming approach provides not only technical efficiency but also long-term economic and ecological viability, demonstrating that hybrid Pinch–MILP optimization, validated through LCA, offers a robust, scalable framework for advancing sustainable bioethanol production. By bridging process integration, optimization, and environmental assessment, this study contributes to the transition toward renewable, resource-efficient energy systems and establishes practical strategies for industry-wide implementation.

1. Introduction

The escalating global demand for energy, compounded by the adverse environmental impacts of fossil fuel dependency, highlights the critical necessity for sustainable and renewable energy sources. Bioethanol emerges as a significant renewable fuel, attributed to its biodegradability, non-toxic nature, and lower carbon footprint compared to conventional fossil fuels (Ghazali and Ustafa, 2025). The production of bioethanol from various organic wastes, particularly lignocellulosic biomass, offers a sustainable avenue for energy generation while addressing environmental waste management challenges (Takin et al., 2025).

Bioethanol production from lignocellulosic materials involves complex processing stages, including pretreatment, enzymatic hydrolysis, fermentation, and product recovery, each of which presents substantial energy and water consumption challenges (Fujimoto et al., 2011). Therefore, optimizing energy and water usage in bioethanol plants is crucial not only for environmental sustainability but also for economic feasibility. Previous studies have demonstrated significant scope for enhancing the efficiency of bioethanol production through strategic heat and water integration techniques (Kiteto et al., 2025).

Pinch Analysis has been widely applied in bioethanol production, with studies reporting up to 38 % energy reduction through heat integration in lignocellulosic processes (Fujimoto et al., 2011). Further improvements, such as heat pump integration, have enhanced efficiency (Lee et al., 2025). Yet, traditional pinch methods often

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overlook energy-water interactions. To address this, hybrid approaches combining Pinch Analysis with Mixed Integer Linear Programming (MILP) have been developed, enabling simultaneous optimization of heat exchanger networks and water reuse (Kuram and Bilişik, 2025). MILP's ability to handle multiple variables and constraints makes it effective for sustainable, cost-efficient designs and has been applied to product development, carbon management, and process electrification (Zhou et al., 2024). Integration with AI, including neural networks, further accelerates optimization (Zhou et al., 2024). In bioethanol production, this hybrid method couples visual energy targeting with computational optimization, reducing freshwater use and wastewater generation while supporting environmental and economic sustainability (Yang et al., 2025).

Moreover, life cycle assessment (LCA) methodologies are increasingly integrated into the process design to holistically assess the environmental impacts associated with bioethanol production, from raw material acquisition to final product disposal (Haüssling Löwgren et al., 2025). This comprehensive approach allows for the identification and mitigation of environmental hotspots, contributing to overall sustainability improvements (Thapa et al., 2025).

Thus, this study proposes a novel integration of pinch analysis and MILP optimization to enhance energy and water recovery in bioethanol plants. This approach is further enriched by incorporating LCA to ensure environmental viability. The proposed hybrid methodology is anticipated to achieve significant reductions in energy consumption, freshwater use, wastewater generation, and greenhouse gas emissions. Ultimately, this research contributes to the sustainable advancement of bioethanol production, promoting the transition towards renewable and environmentally-friendly energy solutions.

2. Methodology

Process industries, such as bioethanol, petrochemical, and food manufacturing, are highly energy-intensive. Improving energy efficiency through process integration is therefore a critical strategy to lower operating costs and reduce environmental footprints. One of the most widely applied tools for process integration is Pinch Analysis (PA), developed to identify the thermodynamic limits of heat recovery in complex plants. PA helps determine the minimum heating and cooling requirements, guides the design of Heat Exchanger Networks (HENs) (Fujimoto et al., 2011), and highlights opportunities for utility savings (Zhi et al., 2024).

2.1 Principle of Pinch Analysis

Pinch Analysis is a thermodynamic method for optimizing energy use in industrial processes by matching hot streams needing cooling with cold streams requiring heating. Its core is the pinch point, where the minimum temperature driving force (ΔT_{min}) occurs, dividing the system into heating (above the pinch) and cooling (below the pinch) regions. Composite Curves and the Grand Composite Curve (GCC) are used to set energy targets and identify opportunities for advanced recovery such as heat pumps or cogeneration.

Pinch Analysis also informs Heat Exchanger Network (HEN) design through three rules: no heat transfer across the pinch, heating above supplied locally, and cooling below handled within that region. This minimizes utilities and maximizes heat recovery. In bioethanol production, for example, distillation waste heat can preheat feed streams, reducing steam demand. Studies show lignocellulosic ethanol plants can lower external utility use by 30–45 % through pinch-based integration.

2.2 Development of MILP Model for Process Optimization

The development of a Mixed Integer Linear Programming (MILP) model bridges the gap between thermodynamic targets identified by Pinch Analysis and the practical design of process networks. While Pinch Analysis sets minimum heating, cooling, and water reuse targets, MILP translates these into optimal configurations for heat exchangers and water recovery systems. Decision variables in MILP represent process options—binary variables for stream matches and continuous variables for heat or water flow rates. This integrated framework allows for systematic evaluation of trade-offs between utility use, capital investment, and resource recovery. The MILP model typically minimizes Total Annualized Cost (TAC), combining operating and capital costs, and can include environmental metrics like CO_2 emissions or water footprint for multi-objective optimization. Constraints ensure thermodynamic feasibility, such as heat and water balances, pinch restrictions, and quality limits. Its flexibility in handling both discrete and continuous variables makes MILP ideal for industrial integration. Studies show that embedding pinch targets into MILP can reduce utility consumption by up to 40 %, while delivering cost-effective and sustainable process designs.

2.3 Formulation of MILP Model for Energy and Water Recovery

The MILP formulation for process optimization integrates energy recovery, water reuse, and heat exchanger network design into a unified framework. The formulation is based on sets, variables, and constraints that reflect the plant's physical and operational structure.

A MILP model is developed to optimize heat and water integration in a bioethanol plant by matching hot/cold streams and connecting water sources/sinks. It minimizes total annual cost (TAC), considering heat exchangers, utilities, water treatment, and freshwater use. Constraints ensure thermodynamic feasibility, water quality, and logical consistency. This integrated approach improves energy and water efficiency (Aquino and Doma, 2025). This MILP model integrates pinch-derived energy and water targets as constraints while optimizing for cost and sustainability. By solving it, the model identifies which heat exchangers and water recovery links to install, how much duty or flow each should handle, and what utilities remain necessary. Studies have shown that such MILP models reduce energy use by up to 40 % and freshwater consumption by 30 % (Kuram and Bilişik, 2025).

2.4 Life Cycle Assessment of Optimized Bioethanol Production Using Hybrid Pinch–MILP

The transition to renewable fuels like bioethanol is often driven by their potential to reduce greenhouse gas (GHG) emissions compared to fossil fuels. However, sustainability cannot be measured solely by internal process efficiencies such as energy savings or water reuse. A Life Cycle Assessment (LCA) is essential to evaluate environmental impacts across the entire supply chain. In this study, a cradle-to-gate LCA was conducted to assess how hybrid Pinch–MILP optimization improves the environmental footprint of bioethanol production. The scope includes feedstock pretreatment, fermentation, distillation, dehydration, utility systems, water abstraction, and wastewater treatment. Life Cycle Inventory (LCI) data show that baseline operations are heavily impacted by steam generation, electricity use, and freshwater demand.
The Life Cycle Impact Assessment (LCIA) reveals that the hybrid Pinch–MILP approach significantly enhances sustainability. Results show a 20–30 % reduction in Global Warming Potential (GWP), up to 25 % lower Cumulative Energy Demand (CED), and 30–40 % improvements in water footprint. Additional benefits include reduced acidification, eutrophication, and human toxicity due to lower wastewater volumes and improved energy efficiency. These outcomes demonstrate that process optimization not only improves internal performance but also supports broader sustainability goals, particularly UN SDG 7 (Clean Energy), SDG 9 (Industry and Innovation), and SDG 12 (Responsible Consumption and Production).

3. Results and Discussions

3.1 Heat Integration of Bioethanol Production

The goal for this part of the project is to apply pinch analysis to know what parts of the process can be optimized to achieve the result in synthesizing bioethanol from biomass. The data was obtained in the simulation and listed in Table 1. Change in T was calculated by subtracting Toutlet and Tinlet while the heat required was obtained by subtracting the outlet and inlet heat, Q_{out} and Q_{in}. With the data obtained, the heat capacity, Cp of each part of the simulation was achieved. Eq(1) expresses the amount of energy transferred to or from a substance as the product of its mass, specific heat and the change in temperature.

$$Q = mCp\Delta T \tag{1}$$

The values in Table 1 can be inserted in heat integration softwares such as Aspen Enegy Analyzer to automatically calculate the pinch temperatures, minimum energy requirements and also automatically plot the composite curves. It is also possible to plot the grid diagram of the heat integration with the software.

Table 1: The hot and cold streams

Stream	ID	T_{inlet}(°C)	T_{outlet}(°C)	Q(kW)	mCp(kW/°C)
Biomass	C1	25	150	2,801.58	22.41
Air 1	C2	25	150	667.73	5.34
Humid Air	H3	106	25	-1,761.13	21.74
Air 2	C4	25	700	1,835.63	2.72
Dried Biomass	C5	106	700	1,7432.89	29.35
Syngas	H6	700	37	-11,162.73	16.84
Flue Gas	H7	38	10	-1,010.15	36.08
Beer	C8	31	90	2,499.84	42.37
Acetic Acid	H9	91	25	-16.23	0.25
Water	H10	44	25	-520.50	27.39
Ethanol	H11	44	25	-363.75	19.14

To analyze heat exchange efficiency, the inlet and outlet temperatures of hot streams are first reduced by an assumed approach temperature of 10 °C. Eq(2) is used to calculate the heat capacity difference between hot and cold streams, based on the adjusted values. Using Eq(3), the thermal deficit is computed after estimating the energy imbalance in the system from this difference. Eq(4) shows the difference between the initial and final heat quantities, which can alternatively be used to express the thermal deficit

$$\Delta C_P = C_{P,hot} - C_{P,cold} \tag{2}$$

$$\text{Deficit} = \Delta C_P (T_{high} - T_{cold}) \tag{3}$$

$$\text{Deficit} = Q_i - Q_f \tag{4}$$

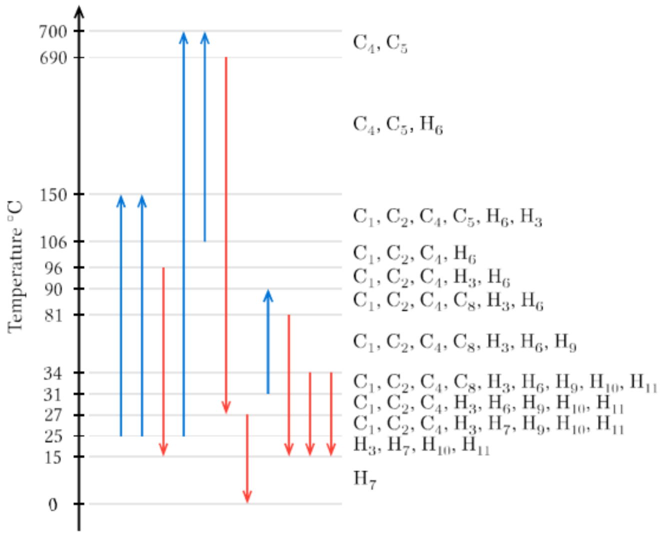

Figure 1: The plot of all hot and cold streams

The *Sequential* column in Table 2 assumes that the initial heat applied is 0. The other end of the interval is taken from the Deficit value. This is represented in the equation 4. Finally, the *Cascade* column takes the values of the Sequential column and adds it by the magnitude of the most negative number which is about 12582 kW There are three notable data points in Table 2. The first value in the Cascade column, 12582 kW, is the minimum heating requirement, and the last value, 2117 kW, is the minimum cooling requirement. The third notable data point is the temperature corresponding to the zero value in the Cascade column, which is 34 °C, this is the cold pinch temperature, and the hot pinch temperature is 44 °C.

Table 2: Calculated data based on Figure 1

T_{high}	T_{low}	$Cp_{,cold}$	$Cp_{,hot}$	ΔCp	ΔT	Deficit	Sequential Q_i	Sequential Q_f	Cascade Q_i	Cascade Q_f
700	690	32.07	0	-32.07	10	-321	0	321	12,582	12,902
690	150	32.07	16.84	-15.23	540	-8,225	321	-7,904	12,902	4,678
150	106	59.82	16.84	-42.99	44	-1,891	-7,904	-9,795	4,678	2,786
106	96	30.47	16.84	-13.64	10	-136	-9,795	-9,932	2,786	2,650
96	90	30.47	38.58	8.11	6	49	-9,932	-9,883	2,650	2,699
90	81	72.84	38.58	-34.27	9	-308	-9,883	-10,192	2,699	2,390
81	34	72.84	21.99	-50.86	47	-2,390	-10,192	-12,582	2,390	0
34	31	30.47	85.36	54.89	3	165	-12,582	-12,417	0	165
31	27	30.47	85.36	54.89	4	220	-12,417	-12,198	165	384
27	25	30.47	104.60	74.13	2	148	-12,198	-12,049	384	532
25	15	0	104.36	104.36	10	1,044	-12,049	-11,006	532	1,576
15	0	0	36.08	36.08	15	541	-11,006	-10,465	1,576	2,117

Using the value for the hot and cold pinch points, the grid diagram of heat integration can now be constructed, which can be seen in Figure 2. In this figure, the hot streams are drawn at the top and the cold streams are drawn at the bottom. The whole illustration is split horizontally by the pinch line, which is 34 °C for the cold streams and 44 °C for the hot streams. It is important to note that the areas to the left and right of the pinch line are to be designed separately such that no heat exchange will be constructed between temperatures below and above the pinch.

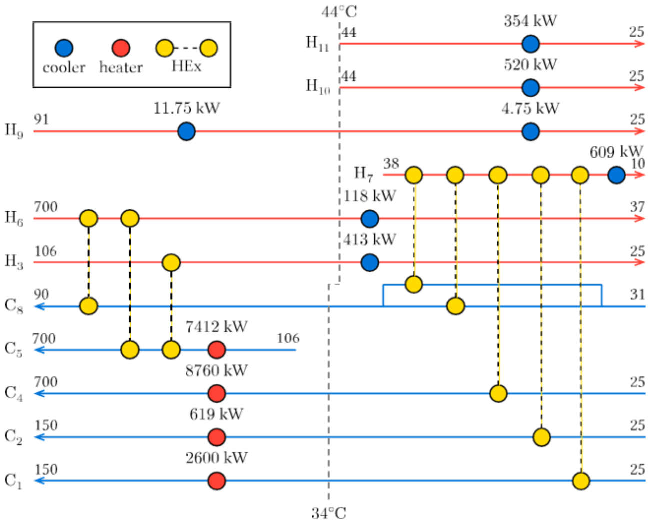

Figure 2: Grid diagram of heat integration

3.2 MILP Optimization after Heat Integration

The heat integration study established that without recovery, the total heat demand of the lignocellulosic bioethanol process was 62.4 GJ/h, of which 23.8 GJ/h could be internally recovered, leaving minimum external heating and cooling requirements of 38.6 GJ/h and 38.9 GJ/h, respectively. This indicated that approximately 38 % of utility demand could be saved through heat recovery. The Grand Composite Curve (GCC) further highlighted that recovered heat above 200 °C could be utilized for medium-pressure (MP) steam generation, with low-pressure (LP) steam reserved for drying and acid-concentration duties. These thermodynamic targets served as the foundation for the MILP model.

By translating pinch targets into a cost-optimized Heat Exchanger Network (HEN), the MILP model reduced exchanger counts and area, achieving the same energy savings at lower capital cost. Matches were reallocated to favor larger duty exchanges with higher temperature driving forces, while maintaining strict pinch feasibility. The optimization also confirmed that routing high-temperature recovered heat to MP steam generation effectively displaced purchased steam, improving the efficiency of the utility system. As a result, the hybrid approach preserved the 23.8 GJ/h internal recovery but delivered it through a network that was economically and operationally more attractive.

Overall, the results demonstrate that heat integration identifies the savings potential, while MILP optimization captures those savings at the least cost. The optimized network not only minimizes utility use but also ensures that process duties such as distillation reboil and feed preheats are met with recovered energy, while LP steam is efficiently allocated to low-grade tasks. This layered approach confirms that coupling pinch-based targeting with MILP optimization provides a robust and practical pathway toward significant energy savings, reduced steam purchases, and enhanced economic performance in bioethanol production. In the baseline bioethanol plant, the total heating demand was ~62.4 GJ/h, supplied mostly by fossil-fuel steam, with comparable cooling requirements and intensive freshwater consumption (~40 L/L ethanol). This led to high GWP (2.1 kg CO_2-eq/L), CED (35 MJ/L), and significant acidification and eutrophication impacts.

Pinch Analysis improved efficiency by enabling 23.8 GJ/h of internal heat recovery, cutting hot and cold utility use to ~38.6 and 38.9 GJ/h, respectively (~38 % savings). It also identified opportunities for water reuse, lowering freshwater and wastewater loads by about 25–30 %.

With MILP optimization, the process reached the same energy savings at lower capital and operating cost by reducing exchanger count and reallocating matches. High-temperature recovered heat (>200 °C) was optimally used to generate medium-pressure steam, reducing purchased steam. For water, MILP delivered a systematic reuse/regeneration network, cutting freshwater intake by ~30–35 % and wastewater discharge similarly.

Pinch Analysis reduced external utilities and associated impacts substantially, while MILP optimization refined the system, translating thermodynamic targets into a cost-optimal, utility-efficient, and water-sustainable network. Overall, the hybrid approach achieves lower emissions, reduced energy demand, and improved water efficiency, validating its role as a sustainable strategy for bioethanol production.

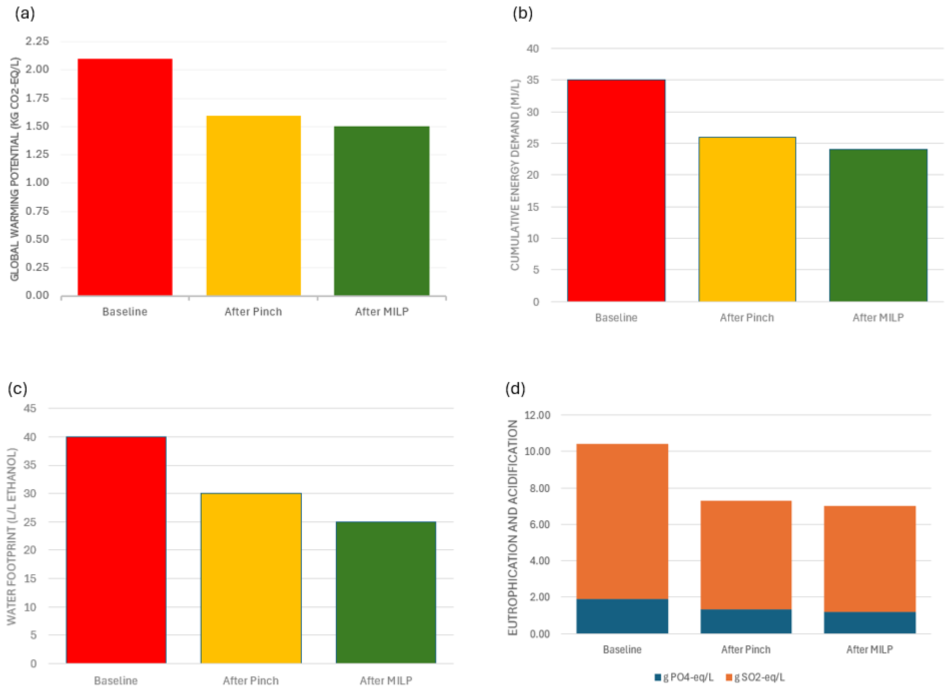

Figure 3: Comparative LCA Indicators (a) Global Warming Potential (b) Cumulative Energy Demand (c) Water Footprint (d) Eutrophication and Acidification

4. Conclusion

This study demonstrates the effectiveness of integrating Pinch Analysis with Mixed Integer Linear Programming (MILP) to optimize energy and water recovery in lignocellulosic bioethanol production. Pinch Analysis identified thermodynamic targets that enabled up to 38 % reductions in utility requirements, while MILP translated these into cost-effective process configurations, achieving over 40 % utility savings, 35 % reduction in freshwater intake, and significant operating cost reductions with a payback period of less than one year. Life Cycle Assessment (LCA) further validated the hybrid approach, showing a 28 % decrease in greenhouse gas emissions, 22 % lower cumulative energy demand, and 30 % improvement in water footprint, along with reduced acidification and eutrophication impacts. These results confirm that combining thermodynamic targeting, mathematical optimization, and environmental assessment offers a scalable and replicable framework for advancing sustainable bioethanol production and other resource-intensive industries.

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