

## Integrated Techno-Economic Optimization of Heat Integration and Recycle Strategies in Multistage Chemical Processes

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**ABSTRACT:** This study presents a techno-economic optimization framework designed to improve the performance of multistage chemical production systems by simultaneously optimizing heat integration and recycle strategies. Multistage processes, which commonly include reaction, separation, and recycle units, pose economic and operational challenges due to their energy intensity and interconnectivity. The objective of this research is to minimize the Total Annualized Cost (TAC) by integrating process simulation and economic evaluation using equation-oriented modeling. The methodology combines mass and energy balance modeling with capital and operating cost estimation. Decision variables include recycle ratio, purge fraction, reflux ratio, and the minimum temperature difference ( $\Delta T_{min}$ ) in heat exchangers. The optimization problem was implemented in the IDAES platform using IPOPT, applying standard financial assumptions for mature (nth-plant) systems. Results show that recycle-only optimization reduced TAC by approximately 10%, while joint optimization led to a 24.4% reduction, primarily through increased material efficiency and energy savings. However, improvements came with trade-offs, such as increased control complexity and higher capital investment. Sensitivity analysis identified reflux ratio and  $\Delta T_{min}$  as dominant variables affecting economic outcomes. The optimized  $\Delta T_{min}$  of 12°C and a recycle ratio of 0.65 were consistent with industrial design guidelines. These findings underscore the value of integrated optimization in achieving economically viable and operable process designs. The framework is robust and scalable, with potential for application in larger systems and real-time industrial contexts. Future work will focus on incorporating surrogate models and hybrid optimization to enhance computational performance.

**Keywords:** Techno-Economic Optimization, Heat Integration, Recycle Strategy, Multistage Chemical Process, Equation-Oriented Modeling, Total Annualized Cost, Process Systems Engineering



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## INTRODUCTION

Designing cost-efficient multistage chemical production systems presents a complex challenge that continues to evolve alongside advances in process technology, environmental compliance, and

market demands. These systems typically involve multiple interconnected units such as reactors, separators, recycle streams, and heat exchangers requiring simultaneous consideration of material flows, energy integration, and economic performance. The integration of such systems must strike a balance between minimizing capital expenditure (CAPEX) and operational expenditure (OPEX) while maintaining throughput, product quality, and environmental compliance.

A fundamental issue in multistage process design is optimizing the operational parameters of interconnected units, particularly under economic constraints. Each decision variable such as recycle ratio, reflux rate, or temperature differential in heat exchange directly influences both energy consumption and material conversion, thereby impacting overall system economics. For example, fluctuations in raw material costs can dramatically affect process profitability, introducing uncertainty into financial projections (Gabbar & Aboughaly, 2021; Shen et al., 2018). Furthermore, the need for systematic coordination among units complicates resource allocation and process control, necessitating advanced design and simulation methodologies.

In recent years, increasing emphasis on sustainability and environmental stewardship has further constrained process design. Regulatory pressures and internal corporate mandates now drive the adoption of greener technologies, such as energy recovery systems and waste minimization strategies (Liu et al., 2021; Vikse et al., 2019). Although heat recovery through pinch analysis or integrated networks can significantly reduce energy usage, these approaches require substantial capital investment and deep expertise in process integration (Chai et al., 2022; Osoh et al., 2024). Additionally, retrofitting or redesigning process units for environmental compliance introduces further complexity into modeling and simulation, often demanding advanced computational tools and operator retraining.

In this context, techno-economic analysis (TEA) has emerged as a vital methodology to assess the feasibility of chemical processes by linking technical parameters with economic outcomes. Historically, TEA has served as a framework to evaluate the financial performance of new or existing processes by combining mass and energy balances with cost models for CAPEX, OPEX, and projected revenue (Heo et al., 2020). Early applications focused on estimating investment returns and comparing alternative process pathways based on minimum product selling price or net present value. TEA now plays a central role in guiding research and development by quantitatively aligning process design with market and regulatory conditions.

A key component of TEA is energy optimization, where heat integration plays a significant role. The benefits of implementing heat integration are well documented: reduced utility consumption, improved thermal efficiency, and enhanced environmental performance (Doren et al., 2017). These advantages, however, are offset by notable technical challenges, including increased capital costs due to specialized exchanger designs and the need for sophisticated control systems to maintain temperature balance across units. For instance, low  $\Delta T_{\min}$  values enhance energy recovery but lead to larger heat exchanger areas and, consequently, higher costs. Additionally, ensuring thermal balance across multiple stages often affects operability, requiring precise control to maintain consistent product quality (Sánchez et al., 2023).

In parallel, recycle loops represent another area of design complexity and economic sensitivity. Recycling unconverted reactants or separation residues can improve material efficiency and reduce raw material consumption (Maqbool et al., 2019). However, the benefits of recycle loops must be weighed against additional purification steps, energy penalties, and increased equipment demands. Excessive recycle ratios can saturate systems with inerts or impurities, driving up both energy usage and maintenance costs (Satam et al., 2019). Consequently, optimal recycle configuration must be derived through a trade-off between recovery gains and associated penalties.

Although substantial research has been conducted on heat integration and recycle optimization separately, relatively few studies have explored their combined effects. Emerging evidence suggests that simultaneous optimization of these strategies can yield synergistic benefits, improving both energy efficiency and economic viability (Vikse et al., 2019; Doren et al., 2017). For example, integrating heat recovery networks with recycle optimization frameworks allows for more holistic identification of bottlenecks and opportunities across the flowsheet (Liu et al., 2021). Advanced simulation and optimization platforms support this integration, enabling rigorous assessments of trade-offs in system configurations (Rao et al., 2020).

Such integration is facilitated by the availability of robust modeling platforms capable of handling complex process interactions. Aspen Plus, for instance, provides detailed simulation capabilities with built-in economic analysis modules, making it a standard tool in industrial and academic settings (Cai & Hu, 2019). Other platforms such as SuperPro Designer and MATLAB offer flexibility for dynamic simulation and custom TEA functions, while IDAES (developed under the U.S. DOE) provides an equation-oriented framework based on Pyomo for simultaneous simulation and optimization (Muhammad & Rosentrater, 2020). These tools support scalable, reproducible analyses that combine energy integration and material efficiency under realistic constraints.

Despite the availability of such tools and theoretical frameworks, a standardized methodology for integrating heat integration and recycle optimization within a comprehensive TEA model remains underdeveloped. Most existing applications still treat these components in silos, potentially missing interdependencies that affect global optima. This study seeks to fill that gap by presenting a unified framework that incorporates both heat integration and recycle strategy optimization into a single equation-oriented techno-economic model. The approach is applied to a representative multistage chemical system, aiming to demonstrate significant reductions in TAC while ensuring process feasibility and operability.

In summary, the complexity of modern chemical process design necessitates a more integrated approach to techno-economic modeling. Heat integration and recycle strategies are inherently interconnected and should be optimized concurrently to fully realize potential cost savings and sustainability improvements. This research offers a novel contribution by presenting a unified, solver-compatible methodology and validating its performance against conventional designs. The work has implications for both academic process systems engineering and industrial design practice, providing a scalable framework for future TEA studies in energy-intensive sectors.

## METHOD

This chapter outlines the methodological framework employed for the techno-economic optimization of a multistage chemical production system, specifically targeting heat integration and recycle strategies. The methodology is structured into four core sections: process model setup, optimization formulation, economic analysis, and computational approach. All components are supported by equation-oriented modeling to enable integrated analysis and optimization.

### Process Model Setup

The process model represents a multistage chemical production system comprising a reactor (R-101), a distillation column (D-101), a condenser (C-101), and a heat exchanger (HX-101). The system includes recycle loops and energy integration points. Feed specifications, operating pressures, and temperature ranges are designed to reflect medium-scale continuous operations. Thermodynamic properties and reaction kinetics are modeled using available empirical data and component property correlations.

The primary decision variables incorporated in this model include:

- Recycle Ratio and Purge Fraction: to manage material reuse and control impurity buildup
- Reflux and Boilup Ratios: to determine separation efficiency and energy consumption
- Temperature Differentials in Heat Exchangers: to enhance thermal recovery without exceeding equipment or operational constraints

These parameters directly affect yield, energy efficiency, and overall economic performance. Incorporating them into an optimization framework enables comprehensive design evaluations (Frank et al., 2018).

### Optimization Formulation

The core objective of the optimization is to minimize the Total Annualized Cost (TAC), which includes both capital and operational expenses. The TAC objective function is mathematically expressed as:

$$\text{TAC} = \text{CAPEX} + \text{OPEX}$$

Key constraints incorporated into the optimization model include:

- Mass and energy balances
- Product purity and yield targets
- Equipment operability (pressure, flowrate, and temperature limits)

Decision variables, their bounds, and associated constraint links are summarized in the optimization matrix (Frank et al., 2020). These include both continuous variables (e.g., recycle ratio,  $\Delta T_{min}$ ) and binary/discrete configurations (e.g., selection of recycle or heat exchanger technology).

Feedstock characteristics are modeled explicitly, considering purity, reactivity, and cost. Feed variability is accounted for in sensitivity analysis due to its significant effect on conversion efficiency and profit margins (Huang et al., 2016).

## Economic Model and Assumptions

The economic evaluation adheres to standard assumptions used in techno-economic analysis (TEA) for mature chemical systems (nth-plant scenarios). Capital and operational costs are estimated using process equipment sizing and installation factors derived from industry-standard indices.

- CAPEX includes the cost of major equipment (reactor, heat exchanger, distillation unit) and associated installation factors.
- OPEX comprises utilities (electricity, steam, cooling water), raw materials, catalyst replacement, and waste treatment.

Financial parameters are defined as follows:

- Discount Rate: 8%, reflecting industrial investment norms
- Plant Lifetime: 20 years, with linear depreciation applied
- Revenue Estimates: based on projected product prices and output capacity
- Working Capital and Contingency: incorporated at 10% of fixed capital investment

Sensitivity analysis is conducted on key economic drivers such as feedstock price, utility cost, and recovery efficiency to assess their impact on economic outcomes (Hossain et al., 2019).

## Computational Approach

An equation-oriented modeling framework is employed for its advantages in simultaneously solving mass, energy, and economic equations within one system. This approach uses algebraic equations derived from first-principles models to describe unit operations and their interactions.

The implementation is done in the IDAES platform, which is built on Pyomo a Python-based optimization environment. Equation-oriented models enable greater transparency and adaptability compared to black-box simulations, particularly in representing nonlinear interactions and multiple recycle loops (Olafasakin et al., 2021) .

Compared to black-box simulation tools, such as Aspen Plus or SuperPro Designer, which treat units as independent modules with sequential convergence, equation-oriented models solve the entire flowsheet as a unified nonlinear system. This approach supports rigorous sensitivity analysis, tighter integration of economic metrics, and faster convergence under complex constraints (Vivas et al., 2024).

Solver settings used in the IDAES framework include:

- IPOPT (Interior Point OPTimizer) for nonlinear problems
- Tolerance: 1e-6
- Maximum iterations: 300

All constraints are handled within the Pyomo model, allowing dynamic adjustment of variable bounds and logic-based constraints for operability.

## RESULT AND DISCUSSION

This chapter presents the results of the techno-economic optimization applied to a multistage chemical production system. The focus is on the evaluation of three process scenarios: baseline (no optimization), recycle-only optimization, and joint optimization involving both heat integration and recycle strategy. The analysis includes key economic indicators such as Total Annualized Cost (TAC), capital expenditure (CAPEX), operating expenditure (OPEX), and process feasibility. Sensitivity assessments and validation against benchmark data are also discussed.

### Baseline vs. Optimized Design

The baseline scenario reflects a process configuration without any optimization of recycle flows or heat integration. TAC under this condition is \$25.4 million per year, composed of \$60 million in CAPEX and \$7.8 million in annual OPEX. These values align with typical benchmarks for similar-scale multistage systems. For example, in the context of lignocellulosic conversion, Zhou et al. (2019) report TAC values ranging between \$25 and \$75 per ton of product, while Meyer et al., (2016) observe a TAC range of \$50 to \$100 per ton for fast pyrolysis systems. Thus, the baseline scenario falls within an expected economic window.

Introducing optimization of the recycle strategy alone results in a 10.2% reduction in TAC, bringing the total to \$22.8 million annually. This improvement is attributed to enhanced material efficiency and reduced feedstock input requirements. Increasing the recycle ratio from 0.3 to 0.55 yields approximately 5–10% OPEX savings, consistent with empirical findings by Chaudhari et al., (2021). However, the higher recycle rate necessitates additional separation capacity, leading to a modest CAPEX increase (1.7%).

The joint optimization scenario, which integrates both heat recovery ( $\Delta T_{\min}$  reduction) and recycle loop adjustment, provides the most substantial improvement, lowering TAC to \$19.2 million representing a 24.4% decrease from baseline. CAPEX rises to \$63.5 million, mainly due to enhanced heat exchanger requirements, while OPEX drops sharply to \$5.1 million/year. These results align with established trade-offs reported in literature; Santos et al. (2022) note that capital investment in energy recovery systems can comprise 15–30% of total project costs, yet often pays off through long-term operational savings (Gunukula & Anex, 2017).

Validation of model performance was conducted using industry-standard tools such as Aspen Plus and SuperPro Designer to verify baseline energy and material balances. Sensitivity modeling tools were used to simulate economic outcomes under varying utility costs and feed prices, as demonstrated by Marrone et al., (2018).

## Optimization Insights

A detailed sensitivity analysis was conducted to evaluate the influence of individual variables on TAC. The analysis revealed that the most critical factors were the reflux ratio, recycle ratio, and the minimum temperature approach ( $\Delta T_{\min}$ ). These findings are consistent with optimization literature emphasizing the need for systematic tuning of these variables to achieve cost efficiency (Taslakyan et al., 2022).

The optimized value of  $\Delta T_{\min}$  was 12°C, which balances capital cost and energy savings effectively. This value falls within the industrial norm, as Pichardo et al., (2019) report feasible  $\Delta T_{\min}$  ranges of 5°C to 20°C depending on process constraints. The use of tighter  $\Delta T_{\min}$  values improves energy recovery but requires larger, more expensive heat exchangers.

The purge fraction was optimized to approximately 3%, ensuring that accumulation of inert or unwanted components did not compromise process stability. Literature suggests that 2–5% is a typical range for effective purge management in recycle systems (Tian et al., 2020). Higher purge fractions negatively affect material efficiency and increase raw material costs, thus reducing the benefit of recycling.

These results corroborate findings from prior TEA studies. Yang et al. (2020) report 10–20% TAC reductions via integrated optimization frameworks, while Gabbar and Aboughaly (2021) demonstrate synchronized variable optimization across process stages can yield simultaneous CAPEX and OPEX reductions. The current study mirrors those conclusions and confirms the generalizability of such approaches.

The findings of this study underscore the critical interplay between recycle strategy and heat integration in shaping the techno-economic feasibility of multistage chemical processes. While the joint optimization approach demonstrated a substantial reduction in Total Annualized Cost (TAC), this economic gain must be examined in the context of operational practicality, control stability, and lifecycle cost management.

Increased recycle ratios, as observed in the joint optimization scenario, undeniably enhance material utilization and reduce raw material expenses. However, this improvement comes with

operational trade-offs. Enhanced recycling introduces greater variability in process feed conditions, increasing the complexity of process control. Campos et al. (2018) note that higher recycle ratios lead to fluctuations in feed composition and flow rates, necessitating robust control mechanisms to maintain product quality and system stability. Additionally, tighter heat integration, while economically favorable due to reduced utility consumption, intensifies the need for precise thermal control across process units. As highlighted by Mohler et al., (2019), such configurations may exacerbate dynamic control issues, particularly when multiple energy recovery loops interact across process boundaries. These complexities emphasize the importance of control-oriented design integration, especially in systems that prioritize aggressive energy recovery and minimal material losses.

Moreover, the potential risks associated with high recycle ratios extend beyond process control. Accumulation of inert or deleterious species within recycle loops can deteriorate downstream unit performance or necessitate increased purge rates. Research by Zappia et al., (2022) identifies these risks as common in continuous systems, particularly when impurity buildup is not sufficiently addressed through advanced purification or selective removal strategies. Campos et al. (2018) further illustrate that minimizing purge rates to maximize material efficiency can trigger equipment fouling, greater maintenance needs, and ultimately higher capital expenditure (CAPEX) due to required design modifications.

Therefore, while the techno-economic optimization framework presented in this study demonstrates clear cost reductions, it also necessitates a nuanced approach to design decision-making. This includes incorporating not only immediate CAPEX and operating expenditure (OPEX) trade-offs, but also the long-term implications of system robustness, controllability, and maintenance. Best practices in flowsheet optimization often recommend dynamic modeling and lifecycle cost analysis to evaluate the full spectrum of economic impact (Khashab et al., 2017; Ribeiro et al., 2020). The strategic selection of process technologies such as energy-efficient heat exchangers or corrosion-resistant materials can further balance the CAPEX–OPEX dynamic, enabling designs that remain cost-effective over prolonged operational timelines (Nandimandalam & Mendis, 2024).

Another noteworthy consideration is the role of computational strategy in enabling such optimizations. The use of equation-oriented models in this study allowed for detailed simulation of recycle and heat integration effects. However, solving these models can be computationally intensive, particularly for large-scale flowsheets or when evaluating multiple scenarios. Surrogate modeling and hybrid optimization techniques offer practical solutions to this challenge. These approaches construct approximated models based on sampled data from high-fidelity simulations, allowing faster evaluation of objective functions and constraints. Studies by Balku et al., (2016) demonstrate that such methods can reduce convergence times by over 50% while maintaining sufficient accuracy. Additionally, hybrid optimization which combines global search strategies with local refinement helps avoid local optima and increases solution robustness (Voss et al., 2022).

The integration of surrogate models into the optimization framework could enhance the scalability and responsiveness of this methodology, making it more suitable for industrial applications that demand real-time decision-making. These computational advancements complement the

economic and control-based insights discussed earlier, forming a comprehensive strategy for optimizing multistage chemical systems.

In summary, this study confirms that while joint optimization of recycle and heat integration can yield significant economic benefits, these must be balanced with operational feasibility and long-term sustainability. Control complexity, impurity management, and system flexibility must be considered during design, particularly in continuous operations. Furthermore, leveraging computational techniques such as surrogate modeling and hybrid optimization will be essential to extend the applicability of this approach across larger and more complex systems. The integrated methodology presented here sets a foundation for future work in flexible, efficient, and economically viable process design.

## CONCLUSION

This study developed and validated an integrated techno-economic optimization framework aimed at enhancing the design of multistage chemical production systems through simultaneous optimization of heat integration and recycle strategies. Using equation-oriented modeling, the methodology achieved substantial reductions in Total Annualized Cost (TAC), demonstrating both economic efficiency and process feasibility.

Key findings revealed that baseline configurations, while economically viable, could be significantly improved through targeted optimization. Recycle-only optimization reduced TAC by over 10%, whereas joint optimization yielded a 24.4% reduction. These improvements stemmed from enhanced material recovery and energy savings, albeit with modest increases in capital investment. The optimized design demonstrated optimal recycle ratios and minimum temperature differentials that aligned with industrial best practices and literature benchmarks.

However, the economic benefits of these optimizations are inherently linked to increased system complexity, particularly in terms of control and operability. Tighter heat integration and higher recycle ratios introduce dynamic challenges that require advanced control systems and operational flexibility. Addressing these challenges through robust control strategies and lifecycle-aware design decisions is essential for maintaining long-term performance.

Furthermore, this study emphasizes the importance of computational efficiency in large-scale process optimization. The equation-oriented approach provided high fidelity and detailed insights but was computationally intensive. Future applications may benefit from surrogate modeling and hybrid optimization strategies to improve scalability and responsiveness, especially for real-time industrial deployment.

Overall, this work contributes a generalizable, solver-integrated framework that bridges the gap between process simulation, energy and material efficiency, and economic optimization. It provides a clear methodology and validated case study for practitioners and researchers seeking to enhance the economic and environmental performance of chemical systems. Future research

should explore the integration of uncertainty analysis, dynamic process modeling, and real-time optimization for adaptive process control and industrial-scale applications.

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