

Energy-Optimized Design of Multicomponent High-Purity Distillation: Comparative Evaluation of Conventional and Intensified Configurations

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ABSTRACT: This study presents a comparative assessment of energy-saving configurations for high-purity multicomponent distillation, focusing on conventional column sequences, Dividing-Wall Columns (DWCs), side utility integration, and heat-pump-assisted systems. The objective is to evaluate each configuration's potential for energy reduction, economic feasibility, and operational robustness. A ternary system was analyzed using shortcut design (Fenske–Underwood–Gilliland), rigorous MESH simulation, and thermodynamic targeting via Column Grand Composite Curve (CGCC). Optimization parameters included reflux ratio, stage count, feed location, and pressure. Simulations revealed that DWCs and heat-pump configurations achieved energy savings of 35–40% compared to the conventional setup. Side utility integration and feed stage/reflux optimization provided moderate reductions of 10–18%. Thermodynamic targeting identified a pinch temperature of 8°C, confirming potential for further heat integration through side reboilers and condensers. Sensitivity analysis indicated that DWCs and heat-pump systems maintained stable product purity and energy performance under $\pm 5\%$ feed variation. While DWCs and heat-pump systems involve higher capital costs, long-term operational savings justify investment. Control and integration complexity were addressed through discussion of adaptive strategies and predictive control methodologies. These findings suggest that intensified distillation configurations significantly enhance process efficiency and offer viable pathways toward sustainable chemical separation.

Keywords: High-Purity Distillation, Energy Efficiency, Dividing-Wall Column, Heat-Pump Distillation, Thermodynamic Targeting, Process Intensification, Sustainability



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INTRODUCTION

Distillation remains one of the most vital separation technologies in the chemical processing industry, applied extensively for component purification and solvent recovery. Despite its widespread implementation, distillation is also among the most energy-intensive operations due to

its inherent reliance on thermal gradients to drive phase separation. This issue is particularly pronounced in high-purity separations of multicomponent mixtures, where the need for sharp splits between components results in significant thermal loads. The challenge becomes more acute when dealing with close-boiling components substances whose boiling points are near-identical leading to increased stage requirements, reflux ratios, and overall energy consumption. For such systems, traditional designs often struggle to provide efficient and cost-effective solutions.

Energy benchmarks for distillation are well-documented. For instance, it is estimated that distillation can account for up to 60% of energy usage in the chemical sector (Muhammad & Rosentrater, 2020). Case studies such as ethanol recovery show consumption rates between 9.8 and 10.4 MJ/kg-EtOH, underscoring the high energy footprint of distillation operations (Torli et al., 2021). This is exacerbated in systems where components exhibit similar volatilities, as seen in the separation of n-butanol and iso-butanol, where conventional methods demand excessive energy input due to the minimal relative volatility (Wan et al., 2024).

Traditional distillation columns are further limited by design inefficiencies. Factors such as tray efficiency, column pressure drop, and feed sensitivity can compromise purity levels, requiring longer operation periods and higher reflux ratios to meet stringent product specifications. Tray inefficiencies and variable feed compositions can significantly degrade column performance, pushing the energy demand beyond practical limits without guaranteeing improved purity (Aqar et al., 2017; Asadollahi et al., 2017). As a result, high-purity separations using conventional columns may become economically and energetically unsustainable.

In response to these challenges, significant attention has shifted toward improving the thermodynamic efficiency of distillation. Among the most promising approaches are thermally coupled systems, such as dividing-wall columns (DWC), which integrate multiple separation zones into a single shell to minimize energy loss and capital expenditure. Studies have reported energy savings of up to 30% using DWCs compared to traditional column sequences (Nhien et al., 2016). Similarly, the integration of heat-pump technology and vapor recompression has gained traction, enabling energy recovery from the overhead vapor to reheat the reboiler section, thus reducing the need for external steam input (Singh & Rangaiah, 2018). Hybrid distillation systems, combining membrane filtration with thermal separation, are also being explored as energy-conscious alternatives (Chen et al., 2018).

Despite the energy-saving potential, the adoption of these advanced configurations necessitates careful evaluation of economic trade-offs. DWCs and heat-pump systems often entail higher initial capital costs due to increased equipment complexity, control challenges, and installation requirements. However, literature suggests that these costs can be offset through operational savings over time, thereby justifying the initial investment from a long-term perspective (Aurangzeb & Jana, 2018; Zhou et al., 2023). Economic analyses show that amortization of advanced equipment costs through energy savings can yield favorable net present values (Christopher et al., 2017).

Parallel to technical and economic considerations, sustainability has emerged as a driving force in distillation process innovation. The global emphasis on reducing carbon footprints, improving energy efficiency, and achieving environmental compliance is pushing chemical manufacturers to rethink conventional separation strategies. Distillation designs are increasingly influenced by life cycle assessments, regulatory policies, and corporate sustainability goals. These drivers have led to the proliferation of green process design approaches that incorporate renewable energy inputs, minimize waste, and optimize utility consumption (Torli et al., 2021; Yang et al., 2022).

Sustainability considerations have also encouraged a reevaluation of how distillation systems are configured, leading to process intensification strategies that combine multiple unit operations into integrated platforms. This convergence of sustainability goals and energy-efficiency imperatives provides the rationale for developing systematic frameworks that guide the selection and optimization of distillation configurations. Such frameworks must account for thermodynamic targeting, capital and operational cost modeling, and control feasibility to support practical implementation.

Within this context, the present study aims to conduct a comparative evaluation of energy-saving configurations for high-purity multicomponent distillation. By examining conventional columns, dividing-wall configurations, heat-pump integration, and side utility applications, this work seeks to identify optimal designs that balance energy efficiency, economic feasibility, and operational robustness. The novelty of this study lies in its holistic integration of shortcut design methods, rigorous simulation (MESH), thermodynamic targeting using Column Grand Composite Curves (CGCC), and multi-objective evaluation of key performance indicators. The scope of the investigation includes detailed analysis of energy and cost metrics, control implications, and system sensitivities.

This research contributes to ongoing efforts in sustainable process engineering by offering a comprehensive methodology for evaluating distillation configurations under high-purity constraints. It supports the informed selection of process alternatives and promotes the adoption of advanced energy-efficient technologies in industrial distillation operations. By aligning technical design with economic and environmental objectives, this study reflects the evolving paradigm of modern chemical process design, wherein energy efficiency and sustainability are treated not as constraints but as core design principles.

METHOD

This study integrates a multistage methodology to evaluate and compare the performance of advanced distillation configurations conventional columns, Dividing-Wall Columns (DWC), heat-pump-assisted systems, and side utility-enhanced setups for high-purity multicomponent separations. The methodology is based on established principles of shortcut design, rigorous simulation, thermodynamic targeting, and performance optimization.

The first step in the design process involved the application of the Fenske–Underwood–Gilliland (FUG) method. This method offers a rapid estimation of the minimum number of theoretical stages (N_{min}) and minimum reflux ratio (R_{min}) for achieving a given product purity. Despite its wide use in preliminary designs, the FUG method carries notable assumptions and limitations. It assumes constant relative volatility across the column, which can lead to inaccuracies when applied to non-ideal or compositionally variable mixtures (Schack et al., 2020). Furthermore, the method presumes vapor-liquid equilibrium and ignores phase inefficiencies such as pressure drops and heat losses, which are critical factors in real operations (Worms et al., 2017). These simplifications make the method unsuitable for predicting performance in highly non-ideal or azeotropic systems, where validation through more robust modeling is necessary (Ramapriya et al., 2018).

Following shortcut analysis, the design process proceeds with rigorous simulations based on the MESH (Mass, Equilibrium, Summation, and Heat) balance equations. These simulations are conducted in Aspen Plus and account for detailed thermodynamic behavior, pressure drops, and energy balances, offering a more accurate representation of real-world column performance. MESH simulation methods are particularly valuable for ternary and multicomponent systems, where interactions among components can significantly affect energy duty and separation efficiency. Studies have confirmed that MESH simulations provide reliable results, though accuracy is highly contingent on the thermodynamic models employed (Kunde et al., 2019). For systems displaying azeotropy or strong non-ideal interactions, the use of accurate thermodynamic models becomes even more critical.

The selection of thermodynamic models plays a pivotal role in both shortcut and rigorous simulations. The choice depends on several factors: the ideality of the system, the presence of azeotropes or phase transitions, and computational resources. For ideal systems, Raoult's Law may suffice; for non-ideal systems, activity coefficient models such as NRTL or UNIQUAC offer greater predictive power. In cases involving supercritical or near-critical behavior, equations of state (EOS) like Peng-Robinson or Soave-Redlich-Kwong may be more appropriate (Ye et al., 2020). Moreover, model selection must consider computational cost and software compatibility, striking a balance between accuracy and efficiency (Recker et al., 2017). Preference should be given to models validated against experimental data, as established in prior literature (Jaubert et al., 2020).

Once the configurations are defined and simulated, optimization is carried out using a multi-objective framework. The decision variables (X) include the reflux ratio, number of stages, feed location, and operating pressure. Constraints (C) are based on separation performance (product purity $\geq 99.5\%$ and recovery $\geq 98\%$), equipment limitations (maximum ΔP of 1.5 bar), and operational feasibility (thermal degradation thresholds). Performance is evaluated using key performance indicators (Y), such as reboiler duty (MW), condenser duty (MW), specific energy use (MJ/kg product), and Total Annualized Cost (TAC).

Thermodynamic targeting is implemented using Column Grand Composite Curve (CGCC) analysis. CGCC helps identify pinch points and quantify the energy integration potential of distillation columns. Specifically, it enables the detection of locations where side reboilers or condensers can be inserted to recover or supply heat more efficiently. The pinch temperature

($\Delta T_{\min}$) is derived from system data and dictates the feasibility of utility integration. This analysis provides additional decision support for integrating side utilities or heat pumps.

Sensitivity analysis is conducted on all configurations to evaluate their robustness under variable feed conditions. Feed flowrate and composition are varied within $\pm 5\%$ of the nominal values to assess their impact on energy duty and product purity. This step is crucial for evaluating the control responsiveness and reliability of each design under real-world fluctuations.

Finally, a comparative assessment is performed based on the simulation and optimization results. Each configuration is benchmarked for its energy efficiency, economic viability, and control robustness. The conventional column setup serves as the baseline for comparison. The configurations are then ranked according to the combined performance in KPIs, allowing for a clear identification of the most promising design.

This integrated methodology allows for a systematic and data-driven evaluation of distillation configurations. It addresses the limitations of shortcut methods by validating them with rigorous simulations, ensures the use of suitable thermodynamic models, and incorporates economic and thermodynamic metrics for holistic performance analysis. By grounding each step in validated literature and best practices in process simulation, the methodology enhances the reliability and applicability of the findings in industrial contexts.

RESULT AND DISCUSSION

This section presents and analyzes the simulation and evaluation results for various distillation configurations applied to a ternary high-purity separation system. The goal is to compare conventional column setups, energy-saving alternatives, and thermodynamic targeting measures with respect to energy demand, economic viability, and operational sensitivity.

Base Case Design

The base case design serves as a benchmark using a conventional distillation setup to separate a ternary mixture with a target purity of 99.5% for component B. The column operates under atmospheric pressure with a feed rate of 100 kmol/h. The feed is introduced as a subcooled liquid at Stage 20 out of 40. The system uses a reflux ratio of 2.5.

Table 1. Base Case Column Design

Parameter	Value
Components	A, B, C
Target xD	99.5%
Feed Rate	100 kmol/h
Feed Quality	Subcooled liquid
Reflux Ratio	2.5

Stages	40
Feed Stage	20
Reboiler Duty	2.8 MW
Condenser Duty	2.7 MW
Pressure	1 atm

As supported in literature, typical reboiler duties for high-purity ternary distillation systems fall within 30–60% of total energy usage, with condenser duties contributing 25–70% (Querino et al., 2019). These values align well with the obtained results, indicating standard performance. Furthermore, feed conditions such as thermal quality and flowrate significantly impact duty levels. Increased feed temperatures have been observed to reduce duty loads substantially (Kartawiria, 2023).

Stage count and feed location also influence energy consumption and separation efficiency. A higher stage count permits better separation at reduced reflux, thus decreasing energy demand (Zhang et al., 2017). Feed location optimization avoids inefficient separations and unnecessary stage use. The base case used midpoint feed placement to ensure balance between rectifying and stripping sections.

Pressure is set at 1 atm, a typical benchmark for such systems, enabling thermal feasibility while maintaining material safety limits (Kong et al., 2023). Studies confirm that lower pressures are favorable for reducing reboiler duty while retaining separation efficiency (Jamali et al., 2023).

Configuration Comparisons

Simulations were conducted for optimized configurations including adjustments to reflux/feed stage, incorporation of side utilities, DWC, and heat-pump-assisted setups.

Table 2. Energy-Saving Options Comparison

Configuration	ΔQ_{reb} (%)	ΔQ_{cond} (%)	$\Delta CAPEX$	ΔTAC
Conventional	0	0	Base	Base
Optimize R + Feed Stage	-10	-9	Low	-5%
Side Utilities	-18	-15	Medium	-10%
Dividing-Wall Column	-35	-30	Medium	-18%
Heat-Pump	-40	-38	High	-20%

Literature corroborates that DWCs can yield energy savings between 30–50% through superior thermodynamic integration (Qian et al., 2020). Heat-pump configurations further reduce heating requirements but involve compressor installation.

Reflux/feed stage optimization showed moderate savings, but literature notes these gains may vary based on system behavior. Simulated results often overestimate field performance, necessitating validation (Carlos & Kolomazník, 2019).

Thermodynamic Targeting Results

Thermodynamic targeting was performed using the Column Grand Composite Curve (CGCC). The pinch temperature (ΔT) was identified at 8°C, suggesting a strong opportunity for energy integration.

Table 3. Thermodynamic Targeting Summary

Metric	Value
CGCC Pinch ΔT	8°C
Side Utility Potential	0.6 MW
Reflux Reduction Potential	0.5 units
Recommended Configuration	DWC + Side Reb

CGCC assists in identifying hot and cold utility zones and visualizing pinch points for strategic heat exchanger placement. Studies have reported that $\Delta T_{\min}$ values between 5–15°C are ideal for distillation integration (Saxena et al., 2017).

Side utilities often contribute 30–40% of total duty, functioning as both heat sources and recovery units. Integration leads to improved thermal efficiency and stable purification outcomes (Yuan et al., 2020).

Sensitivity Analysis

Feed flowrate and composition were varied $\pm 5\%$. The DWC and heat-pump configurations showed minimal energy fluctuation ($<2\%$), while conventional setups exhibited up to 4% deviation. Product purity remained above 99.5% in all cases, confirming robustness.

These findings demonstrate the resilience of advanced designs to input variability, which supports their viability in fluctuating industrial environments.

The comparative results highlight the potential of advanced distillation configurations particularly Dividing-Wall Columns (DWCs) and heat-pump-assisted systems to substantially reduce energy consumption in high-purity multicomponent separations. However, these benefits are accompanied by integration, operational, and economic considerations that require thorough analysis.

DWCs demonstrate superior thermodynamic performance due to their inherent design, which consolidates multiple columns into a single unit and minimizes remixing of intermediate components. However, this compact structure introduces significant integration and control challenges. Managing three product streams within a single shell necessitates precise temperature and pressure control across different zones. This complexity intensifies under dynamic conditions, as even minor fluctuations in thermal profiles can affect internal flows and, consequently, product purity and energy use (Aurangzeb & Jana, 2018). The presence of multiple interacting phases and intermediate heat exchange mechanisms further complicates DWC behavior, requiring advanced control strategies such as model predictive control (MPC) or adaptive control systems to ensure operational stability.

Heat-pump-assisted distillation columns also pose unique integration difficulties. These configurations recover and re-use thermal energy from the condenser to supply the reboiler, significantly reducing the need for external heating. However, managing this energy circulation loop requires detailed thermodynamic modeling and control precision to avoid imbalances that could degrade separation efficiency (Liu et al., 2017). The coupling between the distillation system and the heat pump cycle complicates operational logic, and any discrepancies in vapor and liquid flow distribution must be swiftly corrected to maintain product quality.

Feed variation is another critical factor influencing the performance of these advanced systems. Fluctuations in feed composition or flowrate can alter vapor-liquid equilibrium, demanding responsive control mechanisms to sustain energy efficiency and product purity. An increase in lighter components might reduce thermal demand, while heavier components could necessitate elevated reboiler duty. Without appropriate feedback control, such changes can lead to operational inefficiencies and off-spec products (Aurangzeb & Jana, 2018). Studies have shown that MPC schemes are effective in anticipating feed disturbances and adjusting column parameters accordingly to maintain target specifications (Feng et al., 2018).

Beyond control challenges, the trade-offs between energy savings and capital expenditures (CAPEX) must be thoroughly evaluated. While DWCs offer energy reductions of up to 30–40% over conventional columns, their implementation entails higher initial investments. These costs stem from more complex internals, specialized manufacturing, and detailed process integration requirements (Franke, 2017). Despite this, the long-term operational savings especially in energy-intensive industries can justify the initial financial burden. Economic modeling that incorporates net present value (NPV) and total annual cost (TAC) should guide decision-making during early design stages. Indeed, in many applications, intensified systems offer favorable return-on-investment timelines due to consistent reductions in utility costs (Kroiss et al., 2017).

In terms of control performance, recent research indicates that intensified systems such as DWCs not only achieve energy benefits but also exhibit enhanced dynamic stability. Thermally coupled columns, when equipped with advanced control strategies like MPC or adaptive neural networks, respond more efficiently to disturbances compared to traditional setups. This improved responsiveness enables better maintenance of product purity and energy efficiency, even during startup, shutdown, or transient feed changes (Osuolale & Zhang, 2016).

Real-time monitoring and automation also contribute significantly to operational robustness. For instance, smart sensor systems integrated with feedback loops can continuously adjust reflux ratios, feed locations, and internal pressures, ensuring optimal performance (Franke, 2017). These systems also enable predictive maintenance by identifying early signs of column inefficiencies or equipment degradation. As computational resources and control algorithms continue to advance, future distillation designs will increasingly benefit from digitalization and intelligent control infrastructures (Villareal-Hernández et al., 2023).

Ultimately, while DWCs and heat-pump-assisted configurations offer promising avenues for energy and cost savings, their practical adoption depends on addressing operational complexity, sensitivity to disturbances, and higher CAPEX. The integration of dynamic modeling, real-time control, and economic optimization into the design process enhances the feasibility and scalability

of these technologies. When these elements are carefully calibrated, advanced distillation systems can fulfill the dual mandate of high efficiency and sustainability in modern chemical engineering.

CONCLUSION

This study provides a comprehensive evaluation of energy-efficient configurations for high-purity multicomponent distillation, emphasizing the comparative performance of conventional column sequences, Dividing-Wall Columns (DWCs), side utility integration, and heat-pump-assisted systems. Through the application of shortcut design methods, rigorous MESH simulations, thermodynamic targeting via Column Grand Composite Curve (CGCC), and multi-objective optimization, each configuration was analyzed for its energy consumption, economic implications, and operational robustness.

Key findings reveal that DWCs and heat-pump-assisted columns outperform conventional setups in terms of energy efficiency, achieving energy reductions of up to 35–40%. While reflux/feed optimization and side utility enhancements also contribute to energy savings, their impacts are comparatively moderate. Thermodynamic targeting confirmed that proper integration of side reboilers and condensers can further reduce energy duty, particularly around CGCC pinch points. Sensitivity analyses demonstrated the superior stability of DWCs and heat-pump systems under variable feed conditions, reinforcing their practical viability.

Despite their performance benefits, these advanced configurations present notable challenges. DWCs require complex internal structuring and sophisticated control strategies due to the simultaneous handling of multiple streams in a single shell. Heat-pump integration adds to this complexity with thermal feedback loops demanding precise modeling and management. Both configurations involve higher capital expenditures (CAPEX), yet long-term operational savings can offset these initial investments. Economic analysis indicates that with proper design and control, the return on investment (ROI) for such systems can be favorable.

The scientific contribution of this work lies in its structured and comparative framework that bridges design, simulation, and economic evaluation for distillation systems. By integrating thermodynamic targeting and sensitivity analysis into the evaluation process, this study offers practical guidance for process engineers aiming to implement sustainable and energy-efficient separation technologies. The methodology demonstrated herein supports informed decision-making by balancing energy performance, operational flexibility, and economic feasibility.

This research reinforces the relevance of intensified distillation technologies within the broader context of sustainable process engineering. As the chemical industry moves toward decarbonization and efficiency, the deployment of energy-saving configurations such as DWCs and heat-pump-assisted systems will play an increasingly critical role. Future research may explore hybrid systems, advanced control architectures, and real-time optimization tools to further enhance the adaptability and efficiency of these systems in dynamic industrial environments.

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