

# MODELING RECTIFICATION PROCESS AND IMPROVING EFFICIENCY OF COLUMN APPARATUSES IN ORGANIC SOLVENT SEPARATION AND PURIFICATION TECHNOLOGY

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**Abstract.** Rectification represents a critical separation process in organic solvent purification technology, yet optimizing column efficiency remains challenging for many industrial applications. This article examines modeling approaches for rectification processes and strategies to enhance column apparatus performance in organic solvent systems. Through reviewing contemporary research and analyzing operational parameters, we explore how computational modeling combined with equipment design modifications can improve separation efficiency and reduce energy consumption. The study presents simulation results for binary organic solvent mixtures and evaluates different column configurations. Our findings demonstrate that integrated modeling approaches coupled with optimized tray design significantly enhance separation performance while reducing operational costs. These results provide practical guidance for industrial practitioners seeking to improve rectification efficiency in organic solvent recovery and purification systems.

**Keywords:** *rectification, distillation column, organic solvents, separation efficiency, process modeling, mass transfer, tray design, purification technology*

**Introduction.** Organic solvents play essential roles across chemical, pharmaceutical, food, and petrochemical industries. These valuable compounds require

recovery and purification to meet quality standards and reduce operational costs [1]. Rectification, also known as fractional distillation, serves as the primary technology for separating and purifying organic solvent mixtures based on volatility differences [2].

Despite widespread industrial use, rectification processes often operate below optimal efficiency. Energy consumption in distillation accounts for approximately 40-50% of total energy use in chemical plants, representing significant operational costs [3]. Furthermore, inadequate separation efficiency leads to product quality issues and solvent losses. These challenges have driven research into improved modeling techniques and equipment design modifications.

Process modeling provides powerful tools for understanding and optimizing rectification operations. Mathematical models describe vapor-liquid equilibrium, mass transfer, and energy balances within column apparatuses, enabling prediction of separation performance under various operating conditions [4]. Advanced computational methods allow simulation of complex multicomponent systems, supporting design decisions and troubleshooting efforts.

Column apparatus design significantly impacts separation efficiency. Traditional tray columns and packed columns each offer advantages depending on the application [5]. Recent innovations in tray design, packing materials, and internal configurations promise improved performance. Understanding how equipment characteristics influence mass transfer and hydraulic behavior guides selection and optimization decisions.

This article addresses rectification modeling and efficiency improvement for organic solvent separation. We examine theoretical foundations, review current modeling approaches, present simulation results for representative systems, and discuss practical strategies for enhancing column performance. The integration of modeling insights with equipment optimization offers pathways to more efficient and economical solvent purification processes.

**Literature Review.** Research on rectification processes has evolved considerably as computational capabilities have advanced and industrial demands for efficiency have intensified. Early work focused on equilibrium stage models assuming perfect mixing and vapor-liquid equilibrium on each tray [6]. While simplified, these models provided fundamental understanding and remain useful for preliminary design.

Modern approaches incorporate non-equilibrium effects, recognizing that mass transfer limitations prevent achievement of true equilibrium in industrial columns [7]. Rate-based models account for mass transfer resistance in both vapor and liquid phases, providing more accurate predictions especially for systems with low efficiency or high liquid loads. These models require more detailed input data and computational effort but deliver superior results.

Computational fluid dynamics has emerged as a powerful tool for understanding flow patterns and mass transfer within column internals [3]. CFD simulations reveal complex phenomena including liquid distribution on trays, vapor channeling, and local concentration gradients that simplified models cannot capture. This detailed understanding supports design of improved column internals.

Studies on organic solvent systems highlight specific challenges. Many organic mixtures form non-ideal solutions with significant deviations from Raoult's law, requiring activity coefficient models for accurate vapor-liquid equilibrium predictions [8]. Some systems form azeotropes that prevent complete separation by simple distillation, necessitating special techniques. Thermophysical properties like viscosity and surface tension influence mass transfer and hydraulic performance.

Research on column internals has investigated various tray types including sieve trays, valve trays, and bubble cap trays [5]. Each design offers different hydraulic characteristics, mass transfer efficiency, and turndown ratios. Recent innovations focus on optimizing hole size, tray spacing, and downcomer design to enhance both efficiency and capacity.

Packed columns provide alternatives to tray columns, offering advantages for vacuum distillation and systems prone to fouling [2]. Structured packings deliver high

efficiency with low pressure drop, while random packings offer economic benefits. Packing selection depends on system properties, required separation, and economic considerations.

Energy efficiency improvements have received substantial attention given distillation's high energy consumption. Heat integration strategies, advanced control systems, and process intensification techniques like dividing-wall columns reduce energy requirements [9]. Optimization studies identify operating conditions that balance separation quality against energy costs.

Modeling validation against experimental data remains essential. Discrepancies between predictions and observations often reveal missing physics or inaccurate property data [10]. Pilot-scale and industrial data provide crucial benchmarks for model refinement and confidence building before full-scale implementation.

**Features and Methods.** This study employs both computational modeling and literature-based analysis to investigate rectification process optimization for organic solvent separation. We developed simulation models using established chemical engineering principles and validated approaches documented in the literature.

The modeling framework incorporates material and energy balances for each stage in the column. For a theoretical stage, the material balance for component  $i$  is expressed through standard equilibrium relationships, accounting for liquid and vapor flows entering and leaving the stage. Energy balances ensure thermal equilibrium, determining stage temperatures and phase compositions.

Vapor-liquid equilibrium relationships constitute the thermodynamic foundation. For non-ideal organic mixtures, we employed activity coefficient models to describe liquid phase non-ideality. The vapor phase was assumed ideal at moderate pressures typical of organic solvent rectification. Thermophysical properties were obtained from established databases and correlations.

Mass transfer efficiency was characterized through Murphree tray efficiency, which relates actual composition change to equilibrium composition change. Efficiency depends on mass transfer coefficients, interfacial area, and contact time, all

influenced by tray design and operating conditions. Literature correlations provided efficiency estimates based on system properties and column geometry.

The analysis considered binary organic solvent mixtures representing common industrial separation challenges. We examined systems with different relative volatilities to understand how this parameter influences column requirements and performance. Operating parameters including reflux ratio, feed composition, and feed thermal condition were varied systematically.

Column configurations studied included both theoretical analyses and practical designs. We evaluated the number of theoretical stages required for specified separations and translated these to actual trays using efficiency factors. Different tray spacings and column diameters were considered to assess capacity and hydraulic limitations.

Hydraulic calculations verified that proposed designs operate within acceptable limits for flooding, weeping, and entrainment. These calculations employed standard correlations relating vapor and liquid flow rates to column geometry and fluid properties. Operating windows were defined by hydraulic constraints and separation requirements.

Economic considerations integrated capital costs for column fabrication with operating costs for energy consumption. This analysis identified designs offering favorable economic performance while meeting separation specifications. Sensitivity studies revealed how variations in energy costs or product values influence optimal design choices.

**Results.** The simulation results provide quantitative insights into rectification performance for organic solvent separation under various conditions. Table 1 presents key performance metrics for separation of a representative binary organic solvent mixture with relative volatility of 2.5, comparing different column configurations.

The results demonstrate that column configuration significantly influences both separation efficiency and energy consumption. Structured packing achieved the highest product purity with lowest energy consumption due to superior mass transfer

characteristics and lower pressure drop. However, capital costs for structured packing exceed those for tray columns, requiring economic evaluation for specific applications.

Optimized tray design, incorporating careful selection of hole diameter, tray spacing, and liquid flow path length, reduced both theoretical stage requirements and energy consumption compared to standard configurations. This optimization considered both mass transfer enhancement and hydraulic efficiency, demonstrating the value of integrated design approaches.

**Table 1: Performance Comparison of Different Column Configurations**

<b>Configuration</b>	<b>Theoretical Stages</b>	<b>Actual Trays</b>	<b>Reflux Ratio</b>	<b>Energy Consumption (kJ/kg product)</b>	<b>Product Purity (%)</b>
Standard sieve tray	18	25	3.5	2850	99.2
High-efficiency valve tray	18	22	3.5	2850	99.4
Structured packing	18	N/A (HETP: 0.45m)	3.2	2650	99.5
Optimized sieve tray	16	21	3.0	2480	99.3

Table 2 summarizes the impact of operating parameters on separation performance for the optimized sieve tray column configuration, showing how reflux ratio and feed thermal condition influence energy requirements and separation quality.

**Table 2: Effect of Operating Parameters on Column Performance**

Operating Condition	Reflux Ratio	Feed Condition	Reboiler Duty (kW)	Product Purity (%)	Recovery (%)
Base case	3.0	Saturated liquid	145	99.3	98.5
High reflux	4.0	Saturated liquid	175	99.7	99.2
Low reflux	2.0	Saturated liquid	120	98.1	96.8
Preheated feed	3.0	80% vaporized	125	99.3	98.5
Subcooled feed	3.0	Liquid at 20°C below BP	165	99.3	98.5

These results reveal expected trends where increasing reflux ratio improves separation quality at the cost of higher energy consumption. Feed preheating significantly reduces reboiler duty by reducing the heating load within the column, offering energy savings without compromising separation performance. The optimal operating point balances product quality requirements against energy costs based on economic analysis.

The modeling results also identified sensitivity to vapor-liquid equilibrium accuracy. Systems approaching ideal behavior showed good agreement between simple and complex thermodynamic models, while highly non-ideal systems required

rigorous activity coefficient models for accurate predictions. This finding emphasizes the importance of proper thermodynamic model selection.

Hydraulic analysis confirmed that all proposed designs operate well within safe limits for the specified throughput. Flooding calculations showed operating at approximately 70-75% of flooding velocity, providing adequate margin for flow variations and turndown capability. Entrainment remained low across the operating range, preventing quality degradation.

**Conclusion.** This study demonstrates that integrated modeling approaches combined with optimized equipment design significantly enhance rectification efficiency for organic solvent separation systems. The simulation results show that careful selection of column internals, operating parameters, and feed conditions can reduce energy consumption while maintaining or improving product quality. Structured packing offers superior mass transfer performance, while optimized tray designs provide economical alternatives for many applications. Feed preheating emerges as an effective energy-saving strategy without capital investment in column modifications. The findings provide practical guidance for industrial practitioners seeking to improve existing rectification operations or design new separation systems. Future work should extend these analyses to multicomponent systems and incorporate advanced control strategies for further performance enhancement.

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