

Review on Core Operation Strategies and Frontier Technologies of Multicomponent Batch Distillation

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Abstract

Multicomponent batch distillation, as a core unit operation for the separation of small-batch, multi-variety, high-purity materials, holds an irreplaceable position in the production of fine chemicals, pharmaceutical intermediates, and specialty solvents. However, the issues of low efficiency and high energy consumption caused by dynamic operation have remained unresolved for a long time. This paper comprehensively reviews recent research progress in operational process innovation, heat integration strategies, and intelligent control technologies. At the operational level, structures such as dual-column pressure-swing, dividing wall batch distillation columns, cyclic total reflux, and intermediate vessel/side-stream withdrawal have effectively improved the separation efficiency for azeotropic systems and multicomponent mixtures. At the heat integration level, strategies including heat pump assistance, internal heat integration, and gradual feeding can achieve energy savings of 20%–60%. At the intelligent control level, methods such as model predictive control (MPC), neural networks, and reinforcement learning demonstrate potential in addressing nonlinearity and uncertainty. Nevertheless, industrial implementation still faces bottlenecks including high costs, data scarcity, and decoupling difficulties. Looking forward, efforts should focus on developing lightweight AI algorithms, promoting control process co optimization, advancing heat integration technologies, and constructing cloud based digital twin operation and maintenance systems, so as to drive the transition of batch distillation towards green, intelligent, and efficient operations.

Keywords: Multicomponent batch distillation, Operational strategies, Parameter coordination, Intelligent control

1. Introduction

Batch distillation is an unsteady-state distillation process, characterized by simple equipment, flexible operation, and adaptability to the separation of small-batch, multi-component materials. It serves as a key separation technology in the production of fine chemicals and pharmaceutical intermediates. During the batch distillation process, the composition of materials in the column changes continuously over time. The traditional constant reflux ratio operation is prone to problems such as unstable product purity and deteriorated separation effect in the later stage, while the single variable reflux ratio operation has defects of high regulation difficulty and poor connection with industrial practical operation. At present, the operation strategy of batch distillation in industrial production mostly relies on experience, lacking a systematic optimization approach, which leads to large fluctuations in product purity and high energy consumption. The operational complexity of multi-component batch distillation is much higher than that of binary systems. The core contradictions of the batch distillation operation strategy are reflected in three aspects: first, the difficulty in sorting separation priorities caused by differences in component volatilities, and the precise cutting of intermediate components relies on scientific sequence planning; second, the dynamic time-varying characteristics of the system during the operation cycle, where the concentration field and temperature field in the column evolve in a strong nonlinear manner, making fixed parameters difficult to adapt to the full-cycle requirements; third, the inherent contradiction of multi-objective optimization, which requires the coordinated optimization of energy consumption and cycle under the premise of meeting product purity. In recent years, with the development of thermodynamic modeling, intelligent algorithms, and process intensification technologies, the batch distillation operation strategy has gradually transformed from the traditional experience-based mode to a "model-driven + engineering verification" mode, forming a diversified technical system covering parameter regulation, process innovation, energy-saving optimization, and intelligent empowerment.

This paper focuses on reviewing the core operation strategies and frontier technologies for multi-component separation, and looks forward to future development directions, aiming to provide technical ideas for the optimization and transformation of batch distillation processes in chemical enterprises.

2. Core Operation Strategies of Multicomponent Batch Distillation

2.1 Dynamic Reflux Ratio Regulation Strategy Based on Product Purity

The reflux ratio is a core operational parameter of batch distillation, directly determining separation efficiency and energy consumption. The mainstream regulation methods are constant reflux ratio and variable reflux ratio, which need to be selectively adopted according to product purity requirements and material component properties; a combined mode of "constant reflux ratio + variable reflux ratio" can also be used.

The constant reflux ratio operation is characterized by a constant reflux ratio throughout the process, with advantages of simple control, stable energy consumption, stable equipment operation, and low investment cost. However, its product purity shows a "high in the early stage and low in the later stage" fluctuation trend with the change of still liquid composition, and the yield of qualified fractions is limited. Therefore, it is mainly applied to rough separation scenarios with low purity requirements, such as simple operation conditions including crude solvent recovery, light component removal pretreatment of wastewater, and laboratory and pilot-scale exploration experiments.

The variable reflux ratio operation (usually aiming to maintain a constant composition of the overhead distillate, with the reflux ratio gradually increasing with the operation cycle) effectively makes up for the purity defect of the constant reflux ratio. It can achieve uniform and stable product quality throughout the process, significantly improve the yield of qualified products, and reduce transitional fractions. It is especially suitable for the fine separation of multi-component, azeotropic/near-azeotropic systems, and is widely used in fields with strict purity requirements such as pharmaceutical intermediates, high-purity solvents, and flavors and fragrances. However, this mode has shortcomings such as complex operation and regulation, sharp increase in energy consumption in the later stage, low production efficiency, and high requirements for the automatic control system.

With the improvement of industrial automation level and the growth of energy-saving demand, the combined operation of "constant reflux ratio + variable reflux ratio" has become the current mainstream application strategy. Through the segmented regulation logic of quickly establishing the concentration field in the column with a constant high reflux ratio in the early stage, ensuring product purity with a variable reflux ratio in the middle stage, and optimizing yield with a constant reflux ratio in the later stage, it not only takes into account the operational stability of the constant reflux ratio, but also absorbs the separation accuracy of the variable reflux ratio, effectively balancing operational simplicity, product quality, and energy consumption economy. It has been widely promoted in the industrial production of modern fine chemicals, intelligent distillation equipment, and batch distillation of complex systems.

2.2 Multi-component Stepwise Separation and Cutting Sequence Optimization Strategy

The core difficulty of batch distillation for multi-component materials (3 or more components) is the separation coupling problem when the boiling points of each component are close. Direct extraction according to the boiling point from low to high is prone to component cross-contamination. It is necessary to combine cutting sequence optimization and stepwise separation strategies, and select an appropriate scheme according to the boiling point difference of components and production scale.

2.2.1 Single-column Stepwise Extraction Strategy

This strategy is suitable for the separation of multi-components with a boiling point difference $\geq 10^{\circ}\text{C}$ and small production scale. Its core is to determine the cutting sequence according to the thermodynamic principle of "separating easily separable components first", and sequentially extract light components, intermediate components, and heavy components. The key operational points include: the cutting point is identified by the sudden change of overhead temperature ($\pm 2^{\circ}\text{C}$), combined with online detection of distillate purity by a refractometer for double verification to avoid misjudgment; extraction is suspended at the cutting point, and total reflux operation is performed for 10–20 minutes to remove the residual previous component in the column and avoid cross-contamination; an exclusive reflux ratio is matched during each extraction stage, with a lower reflux ratio in the light component extraction stage and a higher reflux ratio in the intermediate component extraction stage.

2.2.2 Double-column Coupling Separation Strategy

This strategy is suitable for the separation of multi-components with a boiling point difference $< 10^{\circ}\text{C}$ and high

purity requirements. It adopts two towers in series: a pre-distillation tower and a rectification tower. The pre-distillation tower completes the rough separation to remove most of the easily separable light and heavy components, and the rectification tower performs deep separation for the difficult-to-separate intermediate components. Compared with single-column stepwise extraction, this strategy improves product purity, reduces the operational load of a single tower, and enhances the stability of equipment operation. Zhao (2022) utilized the characteristic that the n-heptane-isobutanol system changes from a minimum azeotrope to a maximum azeotrope with increasing pressure, designed a double-column pressure-variable batch stripping-rectification process, and reduced the heat loss of the rectification tower and the operation cost by pre-cooling the feed.

2.2.3 Intelligent Optimization of Cutting Sequence

For systems with 4 or more components, cutting sequence optimization is an NP-hard problem. Sharma and Jogwar (2025) successfully extended the Marginal Vapor Rate (MVR) method from continuous distillation to the field of batch distillation, providing an efficient and practical tool for the cutting sequence optimization of multi-component batch distillation. Compared with traditional sequential simulation, this method has significant advantages in computational efficiency and can accurately identify the separation sequence with optimal energy consumption. This work provides a new idea for the rapid design and optimization of batch distillation processes, and is particularly suitable for intelligent optimization scenarios that require a large amount of computation, such as multi-objective optimization and surrogate model construction.

For the batch extractive distillation process, Hegely (2025) systematically studied the balance between efficiency and accuracy of its optimization methods. He pointed out that genetic algorithm (GA) is usually used for the optimization of batch distillation processes. Although this method has global optimization capability, it requires a large number of dynamic simulations to evaluate the objective function, resulting in extremely high computational intensity; while direct search methods (such as Nelder-Mead simplex method and Box-complex algorithm) have fast convergence speed but are prone to falling into local optima. To integrate the advantages of the two types of methods, Hegely proposed a hybrid optimization strategy, that is, using GA or Latin Hypercube Sampling (LHS) as the global search method to determine the initial point, and then using simplex or complex algorithm for local refinement. Taking the methanol recovery from a five-component industrial waste solvent containing acetone, methanol, tetrahydrofuran, water, and toluene as a case, Hegely conducted a large number of optimization experiments. The results show that the combination of GA and complex algorithm (GA + C) can obtain the highest profit with good result consistency, while GA+S is faster than GA+C but has larger profit fluctuations. For GA+S, the recommended number of GA generations is 5–15, while for GA+C, good results can be obtained even if only 1 generation of GA is run, but the recommended number of generations is 50. The hybrid methods GA +S, GA+C, and LHS+C are always superior to GA alone in optimization performance, showing their significant potential in the efficient optimization of batch distillation processes.

In industrial applications, the intelligently optimized sequence needs to be modified in combination with pilot-scale verification to avoid the disconnection between the optimal solution of the algorithm and the practical feasibility, providing important guidance for the implementation of the algorithm.

2.3 Energy-saving Optimization of Batch Distillation and Multi-dimensional Parameter Synergistic Regulation Technology

As a typical batch operation, batch distillation goes through four core stages: feeding, total reflux concentration, extraction, and still residue discharge. Its total energy consumption is directly related to the timing connection of each stage and the matching degree of operational parameters. The traditional independent regulation mode is prone to energy waste. Therefore, the core of optimization focuses on the timing coordination of "concentration-extraction" and the linkage regulation of multiple process parameters, forming a comprehensive technical scheme with both practicality and energy-saving performance.

In terms of timing coordination optimization, the traditional fixed duration mode of 30–60 minutes in the total reflux concentration stage is broken. The concentration can be ended by adopting the overhead temperature criterion (stabilized at $\pm 0.5^{\circ}\text{C}$ of the light component boiling point), realizing the shortening of total reflux time and the reduction of still heating energy consumption; in the extraction stage, based on the gradient change of light component content in the column, a dynamic load matching strategy is implemented: high extraction rate combined with high heating load is used for rapid extraction in the early stage, the rate and load are gradually reduced in the middle stage to avoid concentration disorder, and low load is maintained for deep separation in

the later stage, realizing the precise matching of timing and energy consumption.

At the level of process parameter coordination, a multi-dimensional regulation system is constructed around "overhead product purity": for the vacuum distillation scenario of thermosensitive materials, the synchronous regulation of overhead vacuum degree and still temperature is adopted to avoid thermal decomposition of materials while ensuring gas-liquid mass transfer efficiency; to balance the sufficiency of mass transfer and the operation cycle, a closed-loop mechanism of "online purity detection - real-time reflux ratio adjustment" is established, and the dynamic matching between distillate purity and reflux ratio is realized through equipment such as refractometers and gas chromatographs, ensuring operational stability and product quality.

3. Innovation and Industrial Application of New Operation Processes

New operation processes break through the bottleneck of traditional single towers through structural intensification or multi-tower coupling. Their core lies in process operation logic, multi-region coordination, and target adaptation. They have achieved pilot-scale amplification and partial industrial application, becoming an important direction for the efficient separation of multi-component batch distillation.

For the Dividing Wall Batch Distillation Column (DWBDC), a new process intensification equipment, Qian Xing (2026) and his collaborators have carried out systematic research work on its dynamic mechanism, structural optimization, advanced control, and comprehensive performance evaluation. Guo *et al.* (2025) established strict dynamic models of the traditional Batch Distillation Column (BDC), Middle Vessel Batch Distillation Column (MVBDC), and Dividing Wall Batch Distillation Column (DWBDC), and conducted strict optimization and comparative analysis of the operating variables of the three structures through the Bayesian optimization algorithm. The results show that DWBDC is significantly superior to the other two configurations in terms of total operation time and economic benefits, and is a superior batch distillation process intensification structure. Furthermore, through dynamic simulation and operation optimization of the strict model, the energy-saving potential of the dividing wall batch distillation column in unsteady-state operation is confirmed again, which can save 63% energy compared with traditional batch distillation and 47% energy compared with the middle vessel tower. In terms of complex tower type and controllability research, the team explored the temperature difference control scheme of the four-product Petlyuk dividing wall tower and Kaibel dividing wall tower, compared the controllability of different structures under dynamic disturbances, and revealed the design difficulties and improvement directions of the complex dividing wall tower control system. At the level of optimization and comprehensive design, the improved particle swarm optimization algorithm and online Kriging model are used to realize the energy-saving optimization and structural synthesis of the dividing wall tower. In summary, the research of Qian Xing's team has constructed a relatively complete research system of dividing wall batch distillation from dynamic simulation, structural comparison, operation optimization, advanced control to reaction coupling application, laying a solid theoretical foundation for the industrial application of this technology.

Cyclic total reflux batch distillation is centered on periodic operations of "total reflux enrichment - non-reflux extraction - cyclic reflux", consisting of three steps: "total reflux concentration - discharge - non-reflux liquid filling", which is repeated cyclically until the operation ends. On the basis of cyclic total reflux operation, Huang *et al.* (2012) proposed a new non-accumulator cyclic total reflux operation mode for the first time. Through the three-temperature control method of non-accumulator cyclic total reflux batch distillation, mathematical simulation results show that the separation efficiency of this new mode is significantly better than that of constant reflux ratio batch operation and one-time total reflux operation of the overhead storage tank. The middle vessel batch distillation adds an intermediate storage tank in the middle of the column, dividing the rectification column into upper and lower sections for independent operation. Sun (2008) systematically studied the batch distillation process with an intermediate storage tank, established a corresponding mathematical model, and analyzed its operational characteristics. Sun *et al.* developed a batch distillation process with an intermediate storage tank and side draw, established a constant molar holdup model of batch distillation with an intermediate storage tank and side draw, solved it by the two-point implicit method, and found through simulation calculation that the batch distillation process with an intermediate storage tank and side draw can save rectification time and has a large load factor. Cui (2004) systematically studied the operational performance and design calculation of the batch extractive distillation process with an intermediate storage tank through a combination of theoretical analysis and experiments. The side draw batch distillation realizes multi-component separation in a single tower by setting a side draw outlet on the rectification tower body.

The above strategies focus on breaking azeotropic constraints, optimizing periodic operation modes, and

enhancing the multi-component processing capacity of a single tower, together forming important technological progress in the innovation of batch distillation operation processes in recent years.

4. Energy-saving Operation Strategies

In recent years, the research on heat-integrated operation strategies of batch distillation has gradually shifted from the exploration of energy-saving potential of a single technology to multi-technology coupling and system integration optimization. Heat pump distillation technology is evolving from traditional steam recompression to all-electric schemes such as flash vapor circulation; heat coupling and dividing wall tower technologies are developing towards deep heat integration with intermediate heat exchangers; and initial breakthroughs have been made in the dynamic controllability of internal heat-integrated rectification towers. Niazi *et al.* (2025) took the dehydration process of the methyl isobutyl ketone (MIBK)-water heterogeneous azeotrope system as a case, proposed a heat integration and process improvement method for batch distillation based on a progressive feeding strategy. The study found that top feeding has higher separation efficiency than bottom feeding, and the decreasing feeding rate curve has better operational performance than the constant rate and increasing rate curves. On the basis of the progressive feeding strategy, the study further proposed a novel and easy-to-implement heat integration and heat recovery strategy, and evaluated its energy-saving potential under different feeding scenarios. The results show that applying this strategy to a batch distillation device with fixed-rate top feeding, the energy efficiency and productivity are improved by more than 47% compared with the traditional batch distillation device equipped with a decanter. This work provides an engineering solution for the heat-integrated operation of batch distillation processes under dynamic and unsteady-state conditions, and has significant practical guiding value.

5. Empowerment of Intelligent Control Technology, Industrial Bottlenecks and Future Directions

In recent years, the in-depth integration of intelligent control technology and batch distillation has become a research hotspot. Through the combination of data-driven and model-driven approaches, it effectively solves the nonlinear, strong coupling, and uncertainty problems that are difficult to be addressed by traditional control strategies, promoting the transformation of batch distillation operation strategies towards "adaptive and self-optimizing". The current core technical directions include: advanced control strategies (such as Model Predictive Control (MPC), Active Disturbance Rejection Control (ADRC)), application of artificial intelligence and machine learning (such as BP, CNN, LSTM neural networks, and DDPG reinforcement learning), digital twin and online monitoring technology, as well as special intelligent control schemes for specific scenarios such as azeotropic distillation and reactive distillation.

Despite the significant progress made in the above technologies, there are still prominent bottlenecks in industrial applications: the high landing cost of intelligent control, with small and medium-sized enterprises facing shortages of data and talents; the multi-region and multi-parameter coupling of new processes, resulting in insufficient adaptability of traditional control strategies; the limited decoupling control accuracy caused by the interaction of multiple operational parameters; and insufficient strategy robustness under multi-source uncertainties, which easily affects the product purity qualification rate.

To address the above bottlenecks, future development needs to focus on four directions: developing lightweight AI algorithms (such as transfer learning and few-shot learning) and industry-shared databases; promoting the integrated optimization of control and process, integrating green development indicators; constructing cloud collaborative platforms and Internet of Things operation and maintenance systems; and using intelligent algorithms to search for the optimal operation sequence with the goals of minimum energy consumption and shortest cycle. In terms of product quality prediction, Chen *et al.* (2023) proposed a soft sensor model for the unsteady-state distillation process based on BP neural network, which optimizes the network using genetic algorithm, sparrow search algorithm, etc., to achieve accurate prediction of product quality in the unsteady-state distillation process. In addition, relevant studies (Hegely 2025) have provided a detailed dataset for the hybrid optimization of batch extractive distillation processes using genetic algorithm and Nelder-Mead simplex method. This dataset aims to maximize process profit, covering seven-dimensional decision variables such as reflux ratio, entrainer feeding rate and position, operation time, and fraction cutting time, which can be used as a benchmark test case for new optimization algorithms or training data for surrogate model construction.

6. Conclusions

The optimization of multi-component batch distillation operation strategies needs to focus on the core industrial production requirements of "stable purity - efficiency improvement - energy reduction", and be selectively adopted according to material properties and production scale to avoid the limitations of a single strategy. Dynamic reflux ratio regulation is the foundation; for high-purity separation, stepwise variable reflux ratio or combined regulation mode is preferred; for multi-component separation, single-column stepwise extraction or double-column coupling strategy should be selected according to the boiling point difference, and total reflux operation at the cutting point is the key to avoiding cross-contamination; energy-saving optimization can be achieved through multiple paths such as heat integration and pressure-variable operation, and the energy-saving potential of multi-strategy coupling is the largest; intelligent control technology provides a new approach for precise regulation under complex working conditions, which can significantly improve operational stability and optimization efficiency.

In the future, with the development of lightweight intelligent algorithms, control-process integration, resilient operation and other technologies, batch distillation will transform towards a more intelligent, efficient, and green direction, continuing to play a core role in fields such as fine chemicals, pharmaceuticals, and special materials, and providing better technical solutions for the separation of small-batch, high-value materials.

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