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A Reproducible Computational Framework for Cascade Configuration and Enrichment Performance Prediction of Electrochemical and COLEX Lithium Isotope Separation Processes for Molten Salt Reactor

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Abstract

Lithium isotope separation is important for molten salt reactor (MSR) and fusion technologies requiring enriched ^{7}Li and ^{6}Li, respectively. This study develops a reproducible computational framework for predicting cascade configuration and enrichment performance of electrochemical and COLEX processes under ideal model assumptions. The framework targets ^{7}Li enrichment from 92.5% to 99.99% using representative single-stage separation factors of 1.040 for electrochemical process and 1.055 for COLEX. A Fenske-type ideal multistage-cascade equation was derived and implemented through computational simulation to predict minimum theoretical stages, cascade configuration, sensitivity response, enrichment performance, and column-wise actual enrichment for both processes comparatively. The framework predicted 171 theoretical stages for electrochemical process and 126 for COLEX. The three-column configurations comprised 12, 43, and 116 stages for electrochemical process and 9, 31, and 86 stages for COLEX. Sensitivity analysis indicated greater stage-requirement response for electrochemical process than COLEX. Under computational perturbation scenarios involving reductions in representative separation factors, the electrochemical separation demonstrated greater enrichment reduction than COLEX. Column-wise actual enrichments were slightly higher for COLEX in column-1 and column-3, whereas electrochemical was slightly higher in column-2. The parameterized framework is reproducible and can generate alternative configurations and enrichment by varying feed composition, target enrichment, or representative separation factor.

1.Introduction

Lithium isotope separation is important for molten salt reactor (MSR) technology, because ^{6}Li has a high neutron absorption cross-section [1], making enrichment of ^{7}Li desirable for reducing parasitic neutron absorption in lithium-containing molten salt. Natural lithium contains approximately 92.5% ^{7}Li and 7.5% ^{6}Li [1], [2] whereas high-purity ^{7}Li requires substantial isotope separation. The separation is intrinsically difficult because of the similar physicochemical properties [2] of the isotopes and the consequently small isotope effect at an individual separation stage. Therefore, high enrichment generally requires multistage separation or cascade configurations, with the single-stage separation factor [3] being a key parameter governing the required separation stages. Various lithium isotope separation methods have been investigated, including chemical exchange, electrochemical separation, ion exchange, solvent extraction, and membrane-based processes [4].

Among these methods, the column exchange (COLEX) process has historically demonstrated effective lithium isotope separation through preferential isotope distribution between lithium-mercury amalgam and aqueous lithium hydroxide phases [5]. Reported single-stage separation factors for COLEX are generally in the range of approximately 1.05 -1.06 [5], [6]. However, its use of mercury presents environmental and safety concerns and has motivated interest in alternative separation approaches [2], [3]. Electrochemical separation provides a mercury-free alternative and has demonstrated measurable lithium isotope fractionation through electrochemical migration and electrodeposition [1], [7]. For the electrochemical process, Zhang et al. reported a separation factor very close to 1.04 in their earlier studies, while later they reported separation factors ranging from 1.033 to 1.054 [2]. Although the single-stage separation effect can be relatively small and dependent on process and operating conditions [1], [7] the cumulative multistage cascades [3] are employed for successive high purity enrichment of ^{7}Li. Therefore, comparison of these processes requires consideration not only of their single-stage separation factors but also of their cumulative effects in multistage cascades.

Mathematical modeling and cascade analysis have previously been applied to lithium isotope separation, including membrane chemical exchange [3] and centrifugal extraction [8] systems. These studies demonstrate the importance of translating single-stage isotope separation characteristics into multistage process performance. However, a common computational framework that comparatively evaluates different separation processes in terms of theoretical stage requirement, cascade stage distribution, sensitivity to separation-factor variation, enrichment performance, and column-wise enrichment remains useful for process-level assessment. Particularly, at high target enrichment, even a modest difference in separation factor can produce a substantial difference in the theoretical stage requirement. Similarly, unfavorable changes in the representative separation factor can alter the enrichment obtained from a fixed cascade.

In this study, a reproducible computational framework is developed to determine cascade configuration and enrichment performance for lithium isotope separation of electrochemical and COLEX processes using an ideal multistage cascade model. A Fenske-type theoretical stage equation is derived from the isotope-ratio formulation and applied to determine the minimum theoretical stage requirement for enriching ^{7}Li from its natural composition (92.5%) to the target enrichment of 99.99%. Because, ^{7}Li enrichment of approximately 99.99% has been identified as necessary for molten salt reactor applications [2], [9]. Literature-reported single-stage separation factors are adopted as representative separation factors, with 1.040 for electrochemical separation and 1.055 for COLEX. The resulting minimum stage requirements and stage distribution demonstrates the required cascade configurations for both processes. Sensitivity analysis and operational enrichment prediction performance show the susceptibility of the both processes, in which sensitivity analysis expresses as stage requirement response and the operational enrichment prediction expresses as enrichment performance. Column-wise actual enrichment exposes the real enrichment data of each columns. The Integrated computational framework simulation can demonstrate the entire cascade configuration and enrichment performance prediction combinedly.

The computational framework is reproducible and can generate alternative new-cascade configurations and enrichment above or below 99.99% target by varying feed composition (x_f), target enrichment (x_p), or representative separation factor (α), although the present study uses 99.99% as its target enrichment, where $x_f < 0.95, and\ x_p > 0.99$.

2. Methodology

This section presents the terminology and conventions, model assumptions, justification for the representative separation factors, and computational framework adopted in the present study. Together, these establish the theoretical background used for the reproducible computational framework for lithium isotope separation cascade configuration and enrichment performance prediction of electrochemical and COLEX lithium isotope processes.

2.1 Terminology and Conventions

Unless otherwise specified, the terminology adopted throughout this study refers to the ideal cascade model developed herein. According to the conventions adopted in this study, the terms stage and cascade denote an ideal

theoretical stage and an ideal counter-current isotope separation cascade, respectively. Similarly, unless otherwise specified, the terms “number of stages” and “stage requirement” refer to the minimum theoretical stage requirement, while integer stage numbers refer to the corresponding upward-rounded stage requirements used for cascade implementation.

Unless otherwise specified, lithium isotope compositions (e.g., nominal 92.5%, 95%, 99% or 99.99% or actual ^{7}Li composition) refer to the mole% ^{7}Li which is numerically equivalent to the isotopic abundance of ^{7}Li. When isotope composition is expressed as a percentage, it is reported as mole%; whereas in equations and simulations, it is expressed as mole fraction. These conventions are used consistently throughout the manuscript.

Computational prediction: In the present study, computational prediction refers to the theoretical estimation of lithium isotope separation performance obtained from the derived ideal multistage cascade equation, representative separation factors, feed composition, and target enrichment under the specified model assumptions. The predicted quantities include minimum theoretical stage requirement, cascade stage distribution, sensitivity analysis, and final ^{7}Li enrichment under specified separation-factor conditions.

2.2 Model Assumptions

To facilitate a systematic and consistent computational evaluation of lithium isotope separation processes, several simplifying assumptions were adopted in the present study. These assumptions provide a consistent theoretical framework for comparing electrochemical and COLEX processes under identical modeling conditions while maintaining computational simplicity.

1. **Ideal Conditions:** In the present study, ideal operating conditions are defined as the set of process conditions under which a single separation stage attains the selected representative separation factor for the respective process. These conditions include pH, applied voltage, Li^{+} ion migration ratio, temperature, electrolyte composition, and other process-specific operating parameters relevant to the separation factor.
2. **Constant feed composition:** Natural lithium is assumed to be the feed composition with a ^{7}Li abundance of approximately 92.5 %, while the target product enrichment is fixed at 99.99 % Li-7 throughout the analysis.
3. **Ideal separation stages:** Each separation stage is assumed to operate under ideal conditions, such that the representative separation factor remains valid for every theoretical stage. Mass transfer resistance and stage inefficiencies are not considered.

4. **Negligible isotope losses:** Material loss, side reactions, isotope decay, or contamination between process streams are assumed to be negligible. All lithium entering the cascade is assumed to participate in the separation process.
5. **Constant representative separation factor for simulation:** For each computational case, the representative separation factor is assumed to remain constant throughout the cascade. Variations in the separation factor are introduced only between different computational scenarios, and during the sensitivity analysis and operational enrichment performance prediction.
6. **Ideal cascade configuration:** The cascade is assumed to operate according to the computational multicolumn configuration with ideal counter-current isotope separation, and each theoretical stage is assumed to achieve the selected representative separation factor under ideal conditions.
7. **Steady-state operation:** The separation process is assumed to operate under steady-state conditions, and transient effects during start-up, shutdown, or process disturbances are neglected.
8. **Engineering and economic factors excluded:** Equipment sizing, capital investment, operating cost, energy consumption, maintenance requirements, and process optimization are beyond the scope of the present computational analysis.
9. **Negligible hydraulic and transport limitations:** Pressure drop, axial dispersion, channeling flooding, concentration polarization, diffusion limitations, and other hydrodynamic effects are neglected. The model focuses exclusively on the influence of the representative isotope separation factor on isotope enrichment.

Under these assumptions, the developed computational model provides a consistent theoretical framework for predicting the minimum theoretical stage requirements, cascade configuration and stage distribution, sensitivity analysis, operational enrichment performance and column-wise actual enrichment.

2.3 Justification of Representative Separation Factors

To enable meaningful comparative computational analysis of the electrochemical and COLEX processes, a representative separation factor was selected for each process. Although experimentally reported separation factors vary with operating conditions and process configurations, representative

baseline values were adopted as constant representative separation factors for the present study.

Justification for Representative Separation Factor of Electrochemical Process ($\boldsymbol{\alpha_{Electrochemical} = 1.040}$)***:***

Reported electrochemical lithium isotope separation factors vary considerably with the electrochemical system and operating conditions. In this regard, Murali et al. reported separation factors ranging from 1.023 to 1.031 for different electrode materials [1] and Zhang et al. reported that using propylene carbonate (PC) as the solvent and $LiBF_4$ as the supporting salt, graphite cathode yielded values close to 1.04 that were consistent with previous studies [2]. Remarkably, Zhang et al. also reported separation factors for the gel electrolyte system and ionic liquid system 1.033 and 1.054, respectively [2] , while computational modeling by the Wild et al. (OSTI/Columbia University group) further demonstrated that the attainable separation factor strongly depends on electrochemical operating parameters [10]. Therefore, considering these reported experimental studies of Zhang et al.'s paper, $\alpha = 1.040$ [2] was selected as a representative separation factor (α) and the baseline value for the present reproducible computational framework for electrochemical process.

Justification for Representative Separation Factor of COLEX Process ($\boldsymbol{\alpha_{COLEX} = 1.055}$)***:***

For the COLEX process, Lewis and Macdonald reported a separation factor of 1.025 for the isotope exchange in the earliest reported counter-current COLEX study [11], and Palko et al. reported that the lithium isotope separation factor was 1.054 and 1.057, when LiCl was dissolved in ethylenediamine (EDA), and propylenediamine (PDA) respectively [5]. In addition, Okuyama et al. reported that the separation factor varies under different operating conditions and was reported over the values ranging from1.028 to 1.085 [6]. Okuyama also reported an isotope separation factor of 1.056 ± 0.001 for the Li(Hg)-LiCl(DMSO) exchange system where DMSO (dimethyl sulfoxide) serves as the solvent for LiCl [6].

Therefore, based on the experimental separation value of Okuyama et al.'s paper, $\alpha = 1.055$ [6] was selected as a representative separation factor based on the report of Okuyama et al. for the COLEX process and adopted as the baseline value for the present reproducible computational framework.

The representative separation factor is therefore treated as the characteristic of single-stage separation performance corresponding to the defined idealized

baseline condition and serves as the principal input parameter for the subsequent computational prediction of stage requirements, sensitivity analysis, cascade configuration, and enrichment performance.

2.4 Computational Framework

The computational Framework adopted in the study was developed to predict the minimum theoretical stage requirement, cascade configuration, sensitivity analysis and enrichment performance prediction. Initially, representative separation factors for the electrochemical and COLEX processes were selected based on the values reported in the literature, while the natural lithium isotope composition was considered as the feed composition. The target lithium-7 enrichment was specified according to the desired product purity for molten salt reactor applications.

Subsequently, the minimum ideal multistage cascade equation derived in this study was applied to calculate the minimum theoretical stage requirement for each separation process under the assumptions described in Section 2.2. The computational simulation was performed assuming constant representative separation factors, minimum theoretical stage requirement and the absence of material losses or side reactions throughout the cascade. The continuous minimum ideal stage requirement was rounded upward to the next integer to obtain the minimum integer number of theoretical stages required to achieve the specified overall nominal 99.99% ^{7}Li target enrichment (details in Section 4.2).

For the cascade configuration and stage distribution, the overall enrichment range was divided into three consecutive incremental enrichment sections following the general sectionalization principles of cascade design described by Benedict et al. [12] (details in Section 5).

In the sensitivity analysis, we investigated the influence of the perturbations of representative separation factors by ± 0.005 for both electrochemical and COLEX processes maintaining all other model parameters constant. The corresponding minimum theoretical stage requirements were computed for each perturbed representative separation factor (details in Section 6).

Operational enrichment performance prediction evaluates the enrichment performance for reduced representative separation factors which may be influenced by unfavorable operating conditions: pH, applied voltage, Li^{+} ion migration ratio, temperature, and electrolyte composition (details in Section 7.1).

In column-wise actual enrichment, the actual enrichments have been investigated for all three columns, since they vary with the nominal boundary enrichments (details in Section 7.2).

In supplementary code and data, all of the codes and resulted simulation graph and integrated data are presented in Google Colab note book with supplied link. The reproduced test results of the Master Code for Integrated Computational Framework are added varying feed composition, product composition or target enrichment and representative separation factors (details in Section 10).

3. Schematic Multicolumn Cascade and Separation Stage Configuration

To facilitate the conceptual understanding of the computational prediction of the present study, a schematic illustration of an ideal multicolumn cascade system and an ideal separation-stage mechanism are presented based on the general principles of isotope cascade theory, multistage counter-current separation, and cascade design concepts [12], [13]. Two schematic illustrations are presented to depict the conceptual multicolumn cascade configuration and the ideal counter-current separation stage for lithium isotope separation.

3.1 Schematic Multicolumn Cascade Configuration

The enrichment range from the natural composition of ^{7}Li (92.5%) to the target enrichment (99.99%) has been divided into three incremental enrichment sections which is consistent with sectionalization theory [12], where 95% and 99% ^{7}Li are the intermediate enrichment nominal value. Thus, our schematic Figure 1 contains three columns.

The term “nominal” is used here to distinguish the specified enrichment boundaries used for cascade configuration from the actual outlet enrichments obtained after integer-stage allocation. The nominal values serve as design targets for assigning the three cascade sections, whereas the corresponding actual outlet enrichments are determined from the subsequent enrichment calculations using the distributed integer stages.

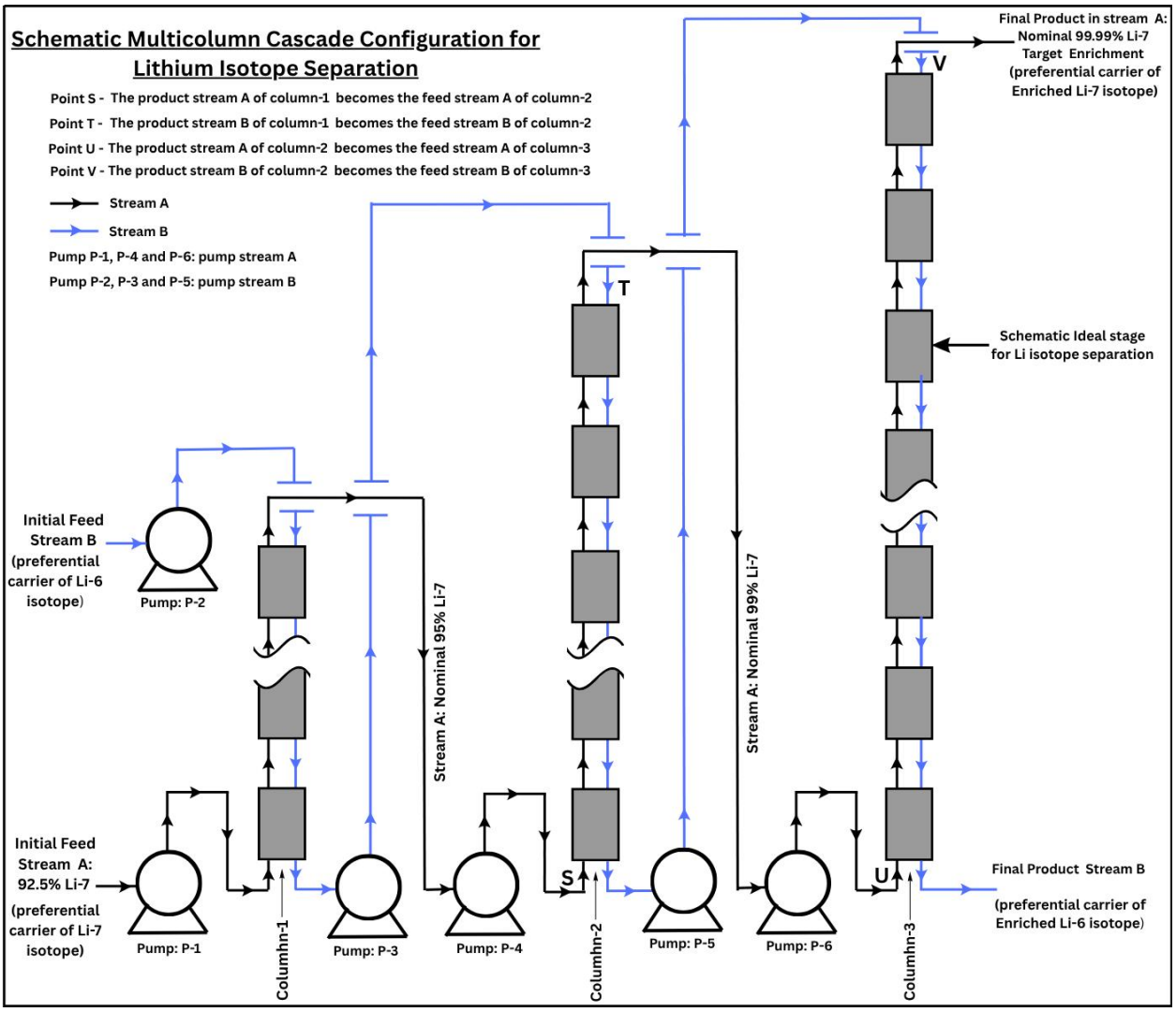

Figure 1. Schematic multicolumn cascade configuration for lithium isotope separation developed by the authors based on the general principles of isotope cascade theory and multistage counter current separation.

Figure 1 presents a schematic multicolumn cascade configuration developed to illustrate the conceptual arrangement of the separation process considered in this study. The ideal cascade configuration is based on the general principles of isotope cascade theory, minimum ideal-stage requirements, multistage counter-current separation, and cascade design concepts which are consistent with the literature reported by Borisevich et al. [13]. In addition, the principles of isotope cascade theory, minimum ideal stage requirements, and cascade design concepts are supported by Song et al. [14]. The schematic diagram is intended solely to illustrate the cascade configuration and flow arrangement;

the actual minimum number of ideal stages in each column is determined from the stage calculations presented in Section 4.2.

In Figure 1, initial feed stream A (preferential carrier of ^{7}Li isotope) is fed into the cascade by pump P-1 as natural isotope composition (approximately 92.5% ^{7}Li) at the bottom-left of the illustration in column-1 and after nominal 95% enrichment in ^{7}Li, the intermediate product stream from column-1 becomes the feed stream A for column-2 through pump P-4 and following the further analogue steps, it becomes the final product of nominal 99.99% target enrichment in ^{7}Li as Final product stream A which is shown in the top-right of the illustration.

Similarly, initial feed B (preferential carrier of ^{6}Li isotope) enters into the top-left of the illustration in column-1 by pump P-2, and becomes the final product stream B, shown in the bottom-right of the schematic configuration, which is enriched in ^{6}Li, but depleted in ^{7}Li isotope. Throughout the cascade, stream A is carried by the pumps P-1, P-4 and P-6, whereas stream B is transferred by the pumps P-2, P-3 and P-5.

3.2 Illustration of an Ideal Counter-Current Isotope Separation Stages

The conceptual illustration of an ideal counter-current separation stages presents a general concept of electrochemical process and COLEX processes.

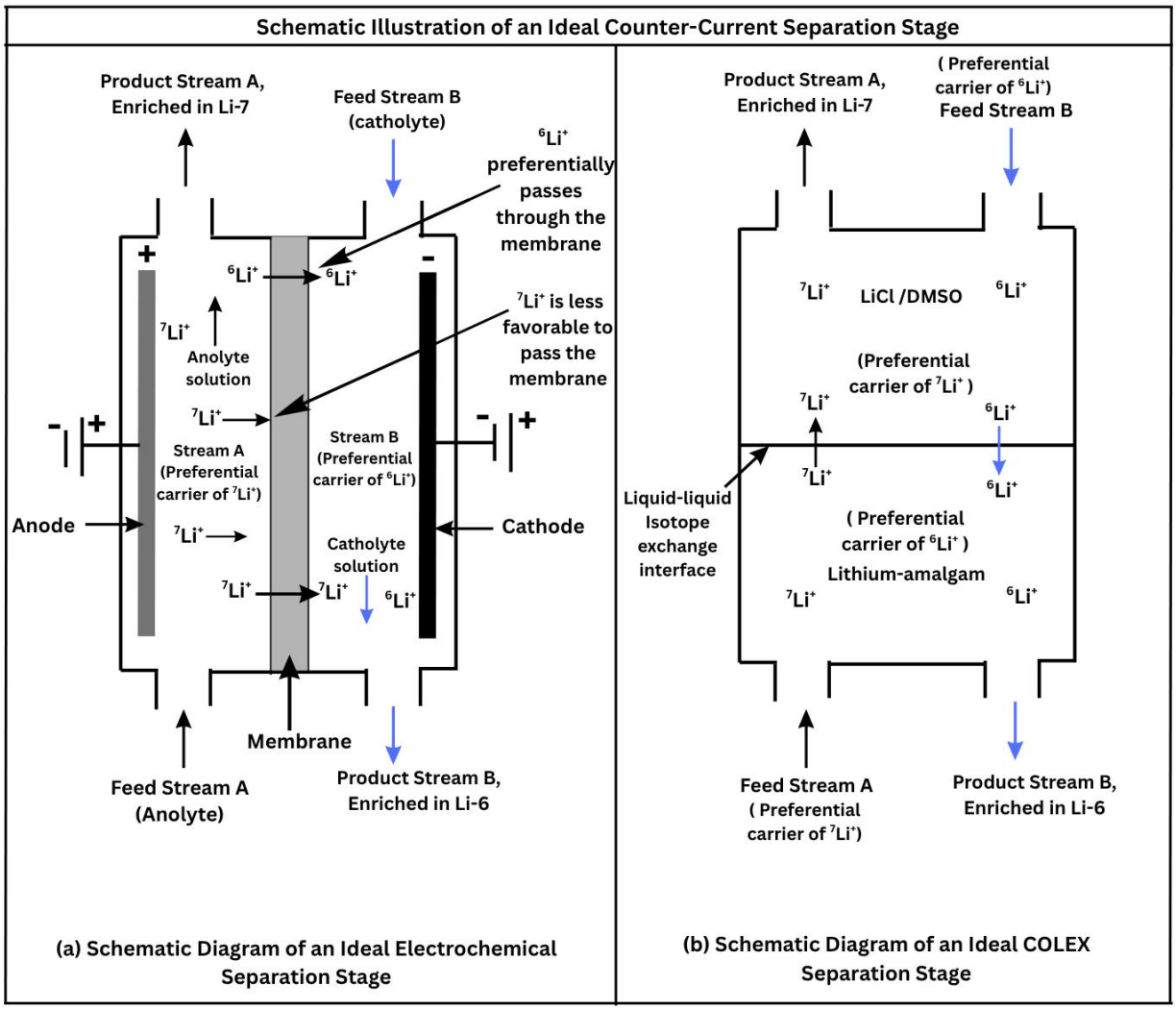

Figure 2. Schematic illustration of an ideal counter-current separation stages for lithium isotope separation developed by the authors based on reported isotope-exchange mechanism and counter-current separation technique.

The ideal counter-current electrochemical separation stage is illustrated in Figure 2(a) based on the general theory of counter-current electromigration presented by Roy et al. [15], and experimental lithium isotope counter-current studied by Okada et al. [16].

In the ion moving mechanism for electrochemical process presented in Figure 2(a), $^7Li^+$ isotope has one more neutron than $^6Li^+$, and both isotopes exhibit differences in their movement through the membrane according to the diffusion process [17], [18]. Consequently, a small fraction of $^6Li^+$ preferentially moves toward the cathode, while $^7Li^+$ remains enriched in the anolyte solution. Although this isotope-selective transport occurs only to a small extent in a

single stage, its effect is progressively amplified through repeated separation in a multistage cascade system, ultimately resulting in higher isotope enrichment [3].

Figure 2(b) schematically represents a single stage COLEX process, in which ^{6}Li and ^{7}Li are exchanged between a LiCl/DMSO solution phase and a lithium-amalgam (Li-Hg) phase under counter-current flow conditions. The counter-current COLEX separation system has been supported by Lewis and Macdonald [11] and also by Giegerich et al. [19].

Figure 2(b) schematically presents a single stage COLEX process, in which ^{6}Li and ^{7}Li are exchanged between an LiCl/DMSO phase and a lithium-amalgam (Li-Hg) phase, corresponding to the Li isotope separation system reported by Okuyama et al. and used to support the representative separation factor (1.055) adopted in the study [6].

In Figure 2 for both processes, the preferential carrier of ^{7}Li, feed stream A enters the stage and undergoes isotope exchange under ideal separation conditions, producing Product Stream A with an increased ^{7}Li concentration. Simultaneously, Feed Stream B flows in the opposite direction and exits the stage enriched in ^{6}Li and correspondingly depleted in ^{7}Li serving as the preferential carrier of ^{6}Li. This idealized separation stage represents the basic theoretical unit of the multistage cascade, where each theoretical stage contributes incrementally to the overall isotope enrichment achieved through successive cascade columns.

The schematic illustrations presented above provide a conceptual representation of the multicolumn cascade configuration and the ideal counter-current separation stage adopted in the present study. They are intended solely to illustrate the conceptual cascade configuration, stage arrangement, and isotope transfer mechanism considered in the computational analysis rather than the detailed design of practical separation units. These conceptual illustrations provide the basis for the computational methodology and the subsequent derivation of the ideal multistage cascade equation.

4. Derivation and Application of an Ideal Multistage Cascade Equation for Lithium Isotope Separation

An ideal multistage cascade equation was derived for lithium isotope separation to determine the minimum theoretical stage requirements for

isotope enrichment processes. The derivation is based on the lithium isotope separation factor (α) and the ideal cascade concept. Although the resulting equation has a mathematical form analogous to the classical Fenske equation, it is formulated for an ideal multistage isotope separation cascade rather than an equilibrium-stage distillation process. The derived equation is subsequently applied to determine the minimum theoretical stage requirements for the electrochemical and COLEX lithium isotope separation processes.

4.1 Derivation of an Ideal Multistage Cascade Equation

For a binary isotope separation system, the separation factor (α) is defined as the ratio of the isotope concentration ratios between the two phases. In the amalgam-solution system, Okuyama et al. (1973) expressed the equation of isotope separation factor (α) as follows

$$\alpha = \frac{(\frac{^7Li}{^6Li})_{solution}}{(\frac{^7Li}{^6Li})_{amalgam}} \quad \text{..... (1) [6]}$$

Equation (1) is rewritten by replacing “solution” with A and “amalgam” with B;

Where, A = principal carrier (preferential carrier) of ^7Li isotope

B = principal carrier (preferential carrier) of ^6Li isotope

So, the Equation (1) becomes,

$$\alpha = \frac{(\frac{^7Li}{^6Li})_{product\ stream\ A}}{(\frac{^7Li}{^6Li})_{feed\ stream\ A}} \text{.....(2)}$$

Borisevich et al. expressed the isotope ratio as, $R = \frac{C}{(1-C)}$ for single-stage ideal cascade [13], where C is the concentration presents in mole fraction.

A schematic configuration of single-stage ideal cascade is presented in Figure-3(a).

According to Borisevich ratio, in this Equation (2),

product ratio in stream A, $R_p = (\frac{^7Li}{^6Li})_{product\ stream\ A} = \frac{x_p}{1-x_p}$;

and feed ratio in stream A, $R_f = (\frac{^7Li}{^6Li})_{feed\ stream\ A} = \frac{x_f}{1-x_f}$.

Where, R_p = Product Ratio in stream A = $\frac{Concentration\ of\ Li-7\ isotope\ in\ product\ A}{Concentration\ of\ Li-6\ isotope\ in\ product\ A} = \frac{x_p}{1-x_p}$

R_f = Feed Ratio in stream A = $\frac{concentration\ of\ Li-7\ isotope\ in\ feed\ stream\ A}{Concentration\ of\ Li-6\ isotope\ in\ feed\ stream\ A} = \frac{x_f}{1-x_f}$

x_p = concentration (mole fraction) of Li-7 isotope in product stream A,

x_f = concentration (mole fraction) of Li-6 isotope in feed stream A.

Here, x_p denotes product fraction or product composition or target enrichment; whereas, x_f denotes feed fraction or feed composition.

Now, the Equation (2) of the separation factor for the single stage isotope separation,

$$\alpha = \frac{\frac{x_p}{1-x_p}}{\frac{x_f}{1-x_f}} = \frac{R_p}{R_f} \quad \text{.....(3)}$$

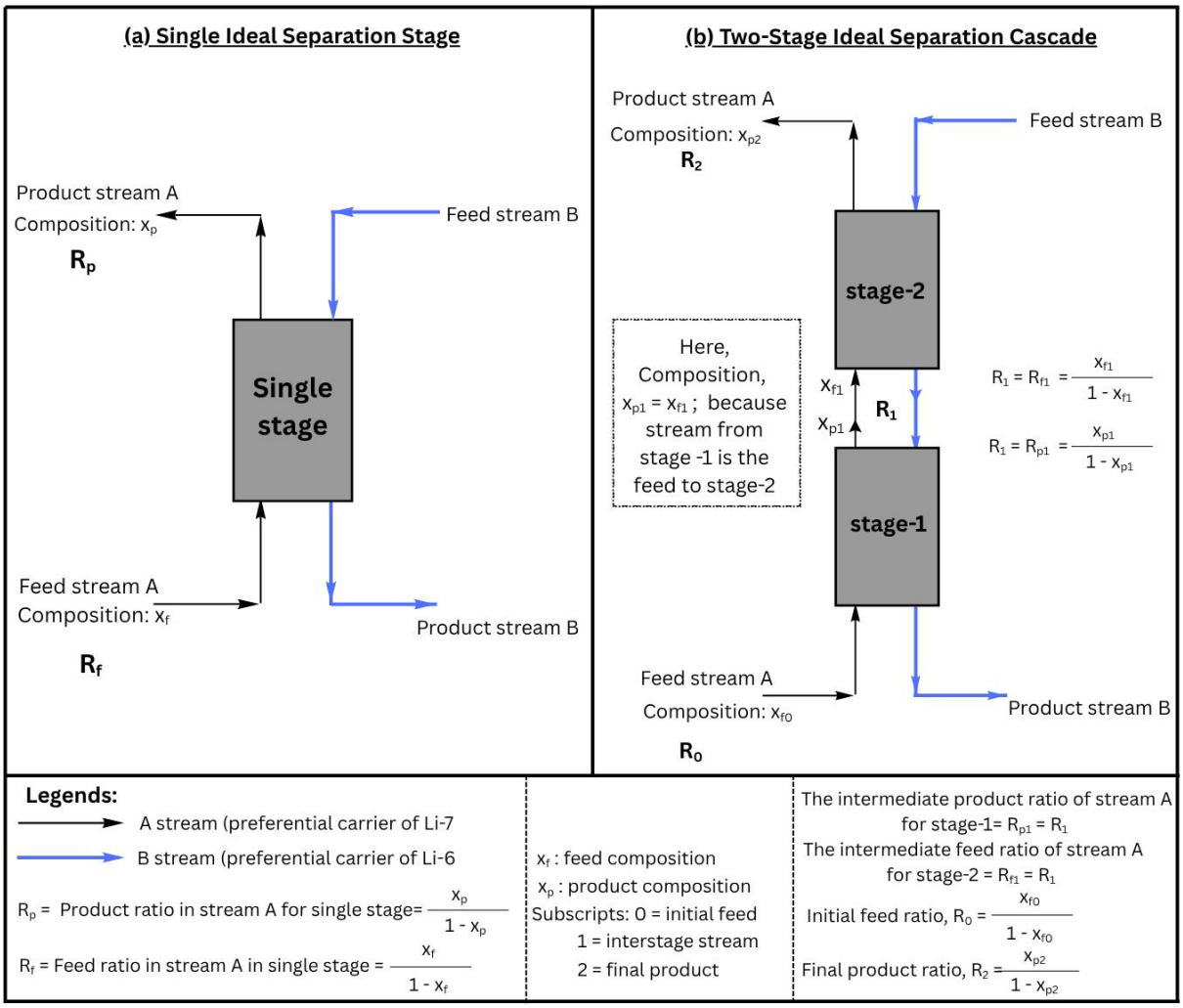

Figure 3. Schematic representation of single-stage and two-stage ideal cascade configurations for ideal multistage cascade equation derivation.

Now, for the two stages cascade, $R_p = final\ product\ ratio = R_2$,

$$R_f = initial\ feed\ ratio = R_0.$$

As illustrated in Figure-3(b), the product stream of stage-1 becomes the feed stream of stage-2, and so,

R_1= intermediate product ratio (R_{p1}) for the stage-1= intermediate feed ratio (R_{f1}) for stage-2.

$$\text{Therefore, } R_1 = R_{p1} = R_{f1} = \frac{x_{p1}}{1-x_{p1}} = \frac{x_{f1}}{1-x_{f1}},\ because, x_{p1} = x_{f1}\ .$$

For the stage-1: $R_1 = \frac{x_{p1}}{1-x_{p1}}$, $R_0 = \frac{x_{f0}}{1-x_{f0}}$ and $\alpha = \frac{R_1}{R_0} = \left(\frac{\frac{x_{p1}}{1-x_{p1}}}{\frac{x_{f0}}{1-x_{f0}}}\right)$.....(4)

Similarly, for the stage-2, $R_2 = \frac{x_{p2}}{1-x_{p2}}$, $R_1 = \frac{x_{f1}}{1-x_{f1}}$ and $\alpha = \frac{R_2}{R_1} = \left(\frac{\frac{x_{p2}}{1-x_{p2}}}{\frac{x_{f1}}{1-x_{f1}}}\right)$.....(5)

Now, assume a single-stage cascade which is equivalent with this two-stage cascade, and produces the same separation performance as the two-stage cascade,

then, $R_p = R_2, R_f = R_0$ and

$$\frac{R_p}{R_f} = \frac{R_2}{R_0} = \left(\frac{R_1}{R_0}\right).\left(\frac{R_2}{R_1}\right) = \left(\frac{\frac{x_{p1}}{1-x_{p1}}}{\frac{x_{f0}}{1-x_{f0}}}\right).\left(\frac{\frac{x_{p2}}{1-x_{p2}}}{\frac{x_{f1}}{1-x_{f1}}}\right) = \alpha.\alpha = \alpha^2$$

[by Equations (4) and (5)]

Similarly, for the cascade system of N number of stages, $\frac{R_p}{R_f} = \alpha^N$ .....(6)

Now, taking the natural logarithm in both sides of Equation (4),

$$\text{we get, } \ln\left(\frac{R_p}{R_f}\right) = \ln(\alpha^N)$$

$$\text{Or, } \ln\left(\frac{R_p}{R_f}\right) = \text{N}\ln(\alpha)$$

$$\therefore N = \frac{\ln\left(\frac{R_p}{R_f}\right)}{\ln(\alpha)} \text{.....(7)}$$

Again, consider a single-stage cascade which is equivalent with this N-stage cascade (N number of stages cascade), and works as equal as the N-stage cascade, then we can get the same result in Li isotope separation, thus from equation (3),

$$\frac{R_p}{R_f} = \frac{\frac{x_p}{1-x_p}}{\frac{x_f}{1-x_f}} \text{.....(8)}$$

Therefore, from Equations (7) and (8), we get, $N = \frac{ln\left(\frac{\frac{x_p}{1-x_p}}{\frac{x_f}{1-x_f}}\right)}{\ln(\alpha)} = \frac{\ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)}$

Finally, the derived ideal multistage cascade equation for determining the minimum theoretical stage requirement

is obtained as, $N = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)}$ .....(9)

for each value of separation factor (α).

Equation (9) represents the final form of the ideal multistage cascade equation which was derived directly from Equations (7) and (8). In our computational simulation, we used Equations (7) and (8) step by step; and for the direct calculation, we applied Equation (9).

4.2 Determination of Minimum Theoretical Stage Requirements

The ideal cascade equation derived in the preceding subsection was subsequently applied to determine the minimum theoretical stage requirements for the electrochemical and COLEX lithium isotope separation processes. The representative separation factors of α = 1.040 and α = 1.055 were adopted based on the reported literature range justified in Section 2.3. Using the natural lithium feed composition (92.5% ^{7}Li) and a target product enrichment of 99.99% ^{7}Li, the minimum theoretical stage requirements were calculated for both processes with the Equations (7) and (8) in computational simulation.

All calculations were performed using computational simulation and are presented in Figure 4 and table 1; the corresponding code is provided in **Supplementary code LHR1** in Section 10. The continuous minimum-stage requirements obtained from the ideal multistage cascade equation were rounded upward to the next integer stage to determine the minimum theoretical stage requirements.

Direct calculation can be done with Equation (9). For example: for the electrochemical process, $\alpha = 1.040, x_f = 0.925, x_p = 0.9999$; then the required minimum stages,

$$N = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)} = \frac{ln\{\frac{0.9999(1-0.925)}{0.925(1-0.9999)}\}}{ln(1.040)} = 170.775 \rightarrow 171, \text{ (for rounding}$$

to the next integer stage).

Next for the COLEX process, $\alpha = 1.055, x_f = 0.925, x_p = 0.9999$;

$$N = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)} = \frac{ln\{\frac{0.9999(1-0.925)}{0.925(1-0.9999)}\}}{ln(1.055)} = 125.100 \rightarrow 126; \text{ (for rounding}$$

upward to the next integer stage).

The electrochemical process yielded 170.775 → 171 stages, while the COLEX process yielded 125.100 → 126 stages; hence, the corresponding minimum theoretical stage requirements were 171 and 126 stages, respectively.

The simulated results presented by Figure 4 and Table 1 indicate that electrochemical isotope separation process requires a minimum of 171 theoretical stages to achieve 99.99% ^{7}Li enrichment, whereas the COLEX process requires only 126 stages under the same enrichment condition. The lower stage requirement for the COLEX process, compared with electrochemical process, is attributed to its higher representative separation factor, which enhances the isotope separation achieved in each ideal stage. The computational simulation predicted that electrochemical process requires 45 more theoretical stages than the COLEX process, corresponding to a relative stage reduction of 26.316% for COLEX compared with the electrochemical process.

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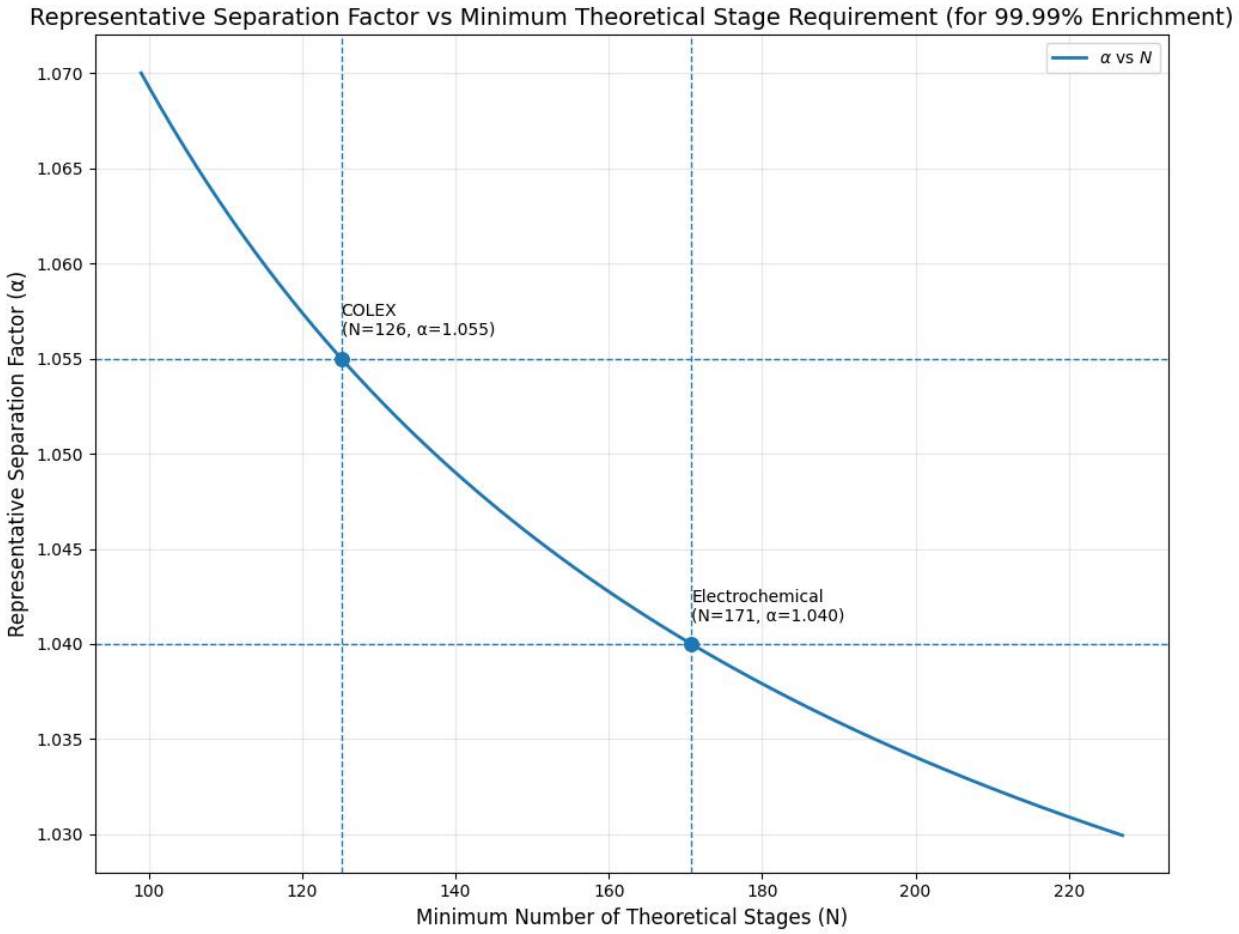

Figure 4. Computational prediction of the minimum theoretical stage requirement as a function of separation factor for achieving 99.99% ^{7}Li enrichment.

Parameter	Electrochemical process	COLEX process
Representative separation factor (α)	1.040	1.055
Target ^{7}Li enrichment %	99.99	99.99
Theoretical stage requirement	171	126
Differences in stages	+45	-
Relative reduction	-	26.316%

Table 1. Comparison of minimum theoretical stage requirements for the electrochemical and COLEX processes at the representative separation factors.

The comparatively lower stage requirement of the COLEX process is attributed to its higher representative separation factor, which enables greater isotopic separation per ideal stage. Consequently, fewer stages are required to reach the specified product enrichment compared with electrochemical process. In contrast, the lower representative separation factor adopted for the electrochemical process results in a more gradual enrichment progression, thereby increasing the total number of theoretical stages required for the same separation objective.

From a process-design perspective, the lower theoretical stage requirement of the COLEX process indicates potentially lower cascade complexity and equipment requirements. Although the present analysis demonstrates the theoretical minimum number of stages under ideal conditions, it provides an important basis for the preliminary design and comparative evaluation of lithium isotope enrichment cascades.

5. Cascade Configuration and Stage Distribution

Cascade configuration was performed to evaluate the distribution of theoretical stages within the proposed multicolumn cascade using the representative separation factors of the electrochemical and COLEX processes. Computational simulations were carried out based on the ideal multistage cascade equation derived in Section 4.1, and the representative separation factors selected through justification in Section 2.3.

A stepwise cascade-design approach was adopted, in which the overall enrichment objective was divided into three nominal incremental enrichment sections as first enrichment section: 92.5-95 mol%, second enrichment section: 95-99 mol%, and third enrichment section: 99-99.99 mol% ^{7}Li. This sectionalized cascade-design approach follows the general principles of multistage isotope-separation cascade design described by Benedict et al. [12], while the specific intermediate enrichment boundaries were selected as computational design points for the present prediction analysis.

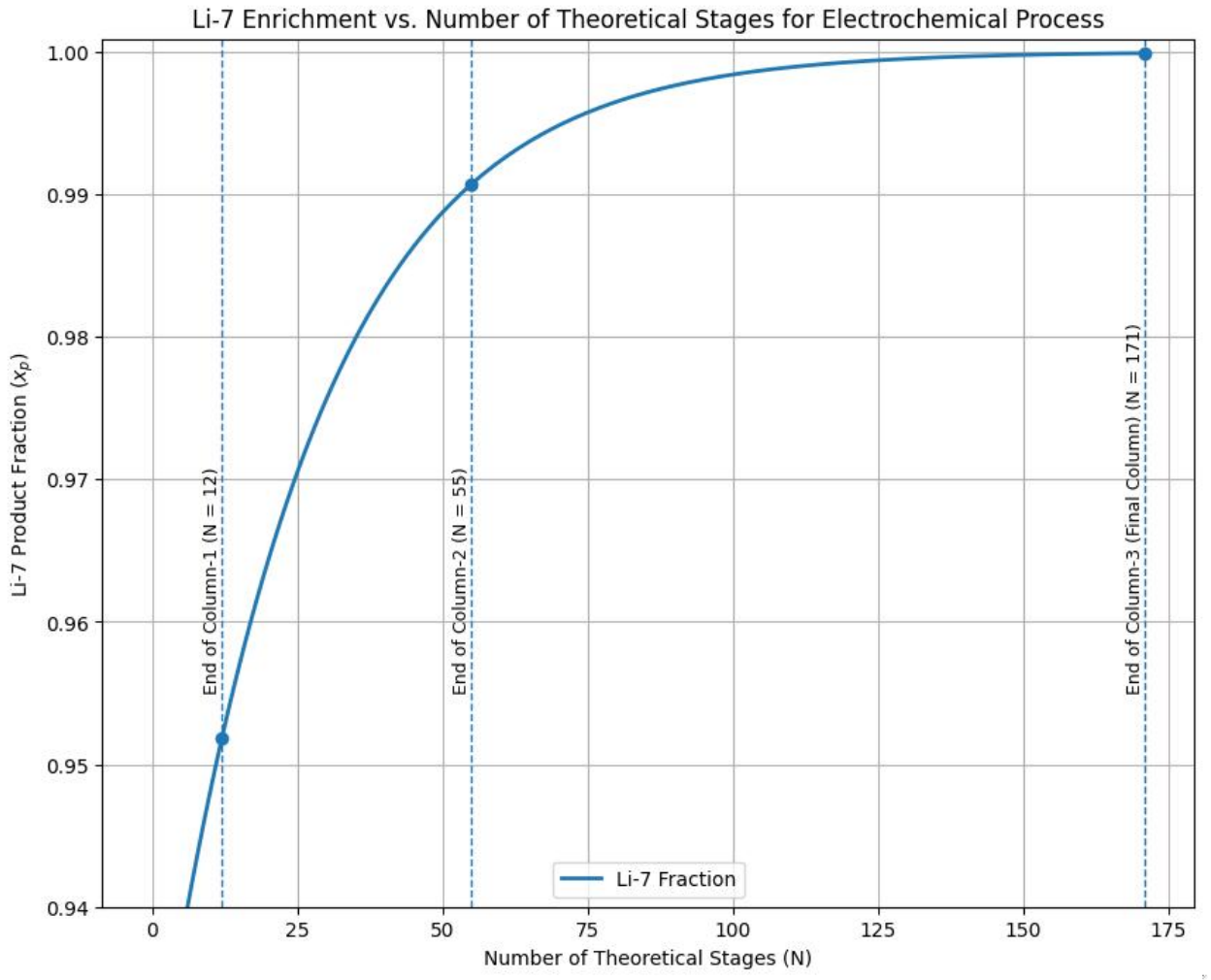

Figure 5. Simulated ^{7}Li enrichment profile and cumulative theoretical stage distribution for the electrochemical cascade system.

These ranges were adopted as design boundaries for stage distribution and do not represent the exact outlet enrichments obtained after integer-stage allocation. Accordingly, column-1 was assigned to the first enrichment section, column-2 to the second enrichment section, and column-3 to the third enrichment section. The actual outlet enrichment of each column was subsequently determined from the sequential application of the allocated integer stages. Because the stage numbers were rounded to integer values, the actual outlet enrichments may differ slightly from their nominal upper boundaries.

According to this three-column cascade configuration, 95% and 99% are adopted as fixed nominal intermediate enrichment boundaries. As a result, the computation framework is applicable to feed composition of ^{7}Li satisfying $x_f <$

0.95 and target enrichment composition of ^{7}Li satisfying $x_p > 0.99$, such that the enrichment can proceed sequentially through the three columns from x_f to x_p:

$$x_f \rightarrow Column\ 1 \rightarrow 0.95 \rightarrow Column\ 2 \rightarrow 0.99 \rightarrow Column\ 3 \rightarrow x_p$$

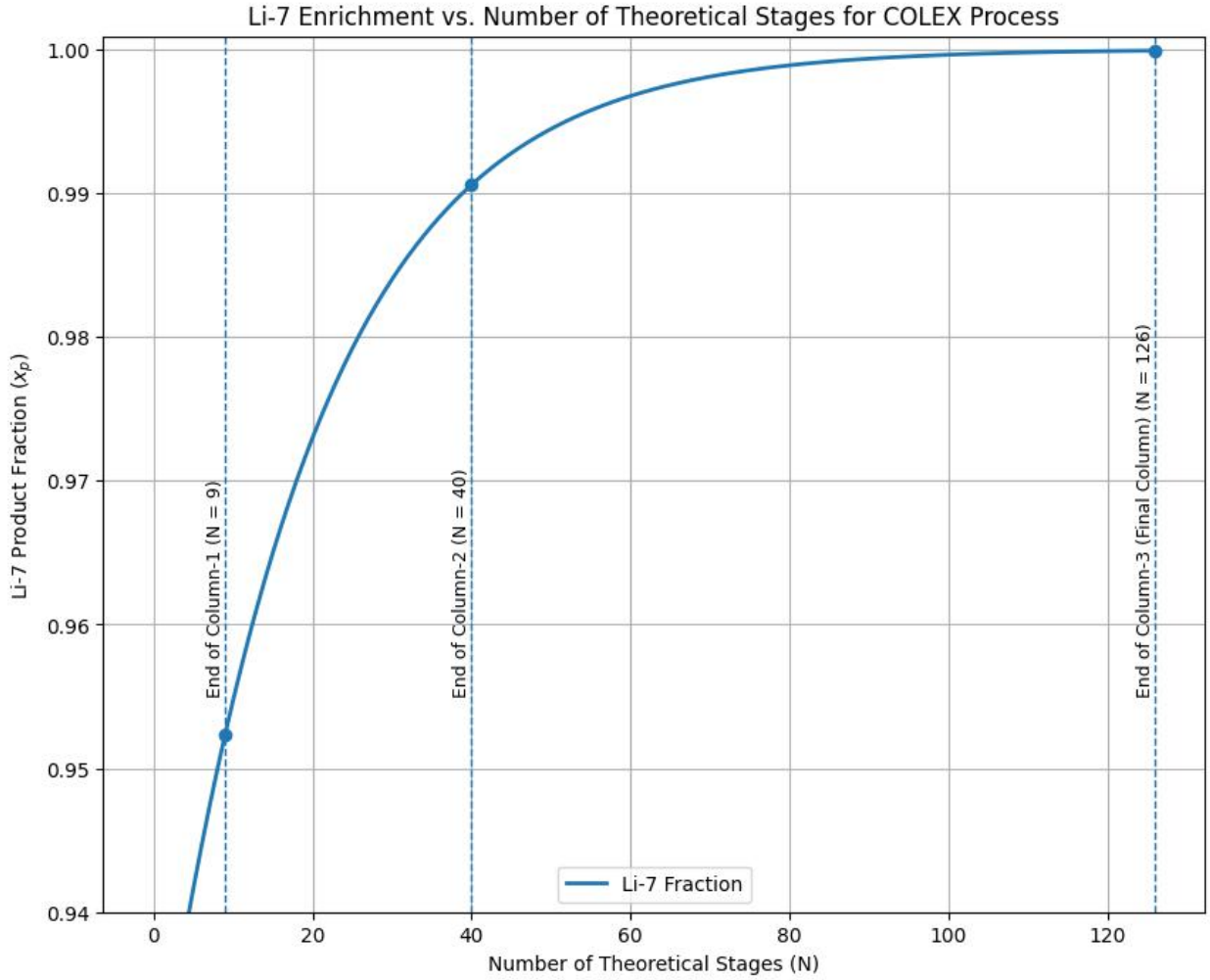

Figure 6. Predicted ^{7}Li product enrichment as a function of the number of theoretical stages for the COLEX process. The highlighted points represent representative cascade designs.

Process	Representative separation factor (α)	Total theoretical stages (N)	Column-1	Column-2	Column-3	Cascade size
Electrochemical	1.040	171	12	43	116	Larger
COLEX	1.055	126	9	31	86	Smaller

Table 2. Numerical distribution of theoretical stages for the conceptual multicolumn cascade configurations for electrochemical and COLEX processes based on the representative separation factors adopted in the study.

All calculations were performed using computational simulation using equation (7) and (8) derived in Section 4.1, and the results are presented in Figure 5, Figure 6 and table 2; the corresponding code is provided in **Supplementary code LHR1** in Section 10.

The simulation results indicate that the electrochemical process requires a total of 171 theoretical stages, whereas the COLEX process requires only 126 theoretical stages to achieve the target 99.99% ^{7}Li enrichment. The corresponding stage distributions and enrichment profiles provide the basis for evaluating the cascade configuration and comparing the design characteristics of the two separation processes

The continuous stage requirements for column-1 and column-2 are rounded upward to the nearest integer stage, and for column-3 the required stage number is then determined as the residual of the total stage requirement.

Accordingly, let, $N_1, N_2, and\ N_3$ denote the theoretical stage requirements allocated to column-1, column-2, and column-3, respectively; and then the total theoretical stage requirement, $= N_1 + N_2 + N_3$; and the required stages of column-3, $N_3 = N - (N_1 + N_2)$ is the residual of the total stage requiement rather than being independently rounded upward. This procedure preserves the minimum total number of theoretical stages while distributing them among the three nominal enrichment sections.

The calculation also can be performed directly with Equation (9). For example: for electrochemical process required theoretical stage distribution using, $\alpha = 1.040,\ x_f = 0.925,\ x_p = 0.950$ for column-1,

$$N_1 = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)} = \frac{ln\{\frac{0.950(1-0.925)}{0.925(1-0.950)}\}}{ln(1.040)} = 11.018 \rightarrow 12 \text{ for rounded to the next integer;}$$

using, $\alpha = 1.040,\ x_f = 0.950,\ x_p = 0.990$ for column-2,

$$N_2 = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)} = \frac{ln\{\frac{0.990(1-0.950)}{0.950(1-0.990)}\}}{ln(1.040)} = 42.087 \rightarrow 43 \text{ for rounded to the next integer;}$$

and for column-3, the residual $N_3 = N - (N_1 + N_2) = 171 - (12 + 43) = 116$.

Although theoretical stage count of column-3 would be,

$$N_3^{'} = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)} = \frac{ln\{\frac{0.9999(1-0.990)}{0.990(1-0.9999)}\}}{ln(1.040)} = 117.670 \rightarrow 118,$$ we rejected it.

Because, if the third section requirement were independently rounded upward, it would give 118 stages, resulting in a total of 12 + 43 + 118 = 173 stages which exceeds the theoretical total stage requirement of 171. Therefore, the column-3 enrichment stage number was assigned as the residual of 116 stages.

Similarly, for COLEX process we got required theoretical stage distribution using $\alpha = 1.055$,

$$N_1 = 8.071 \rightarrow 9;\ N_2 = 30.830 \rightarrow 31;$$

$$\text{and } N_3 = N - (N_1 + N_2) = 126 - (9 + 31) = 86 \ .$$

For the electrochemical process, the data of stage distribution is presented in Figure 5 and Table 2, Column-1 required 12 stages, while the cumulative stage requirement at the end of Column-2 was 55 stages, and at the end of column-3 was 171 stages. Therefore, Column-2 itself required 43 stages, and column-3 required 116 stages.

Similarly, for the COLEX process, the stage distribution data is presented in Figure 6 and Table 2, Column-1 required 9 stages, while the cumulative stage requirement at the end of Column-2 was 40 stages, and at the end of Column-3 was 126. Therefore, Column-2 itself required 31 stages, and Column-3 required 86 stages.

From the simulation result presented in Table 2, it is obvious that with the higher representative separation factor the simulation predicted fewer theoretical stages, whereas with the smaller representative separation factor the simulation predicted a greater number of theoretical stages. Since the representative separation factor of the COLEX process ($\alpha = 1.055$) is larger than that of the electrochemical process ($\alpha = 1.040$), the COLEX process requires fewer theoretical stages (N = 126) than electrochemical process (N = 171).

Similarly, the distributed stage numbers of Column-1, Column-2 and Column-3 of COLEX process are 9, 31, and 86 which are fewer than those of electrochemical process (12, 43, and 116, respectively). Furthermore, the stage distribution among the three cascade columns indicates that for the final enrichment in column-3 (to enrich from 99% to 99.99% ^{7}Li) accounts for the largest proportion of the total stages in both processes, highlighting that achieving ultra-high ^{7}Li purity is the most demanding step of the enrichment cascade. These findings provide valuable insights into cascade design and process optimization for high-purity lithium isotope production in advanced nuclear energy applications.

6. Sensitivity Analysis of the Ideal Cascades with Representative Separation Factor Perturbations

In the present study, the sensitivity analysis was performed for the ideal cascades constructed from multiple ideal separation stages operating under the ideal conditions defined in model assumptions 1 and 3 in Section 2.2.

The representative separation factors were perturbed by ± 0.005 to evaluate the influence of variations in the representative separation factor on the minimum theoretical stage requirements of the electrochemical and COLEX lithium isotope separation processes. Therefore, the representative separation factors were varied by ± 0.005 around the baseline values ($\alpha = 1.040$ for the electrochemical process and $\alpha = 1.055$ for the COLEX process), and the corresponding stage requirements were calculated using the ideal multistage cascade Equations (7) and (8), derived in Section 4.1 through computational simulation (presented in figure 7). All calculations were performed using computational simulation and the results are presented in Figure 7 and table 3; the corresponding code is provided in **Supplementary code LHR1** in Section 10. The continuous stage requirements were rounded upward to the next integer stage, and the minimum theoretical stage requirement consistent with Section 4.2.

The simulation graph consists of two regions corresponding to the electrochemical and COLEX processes. The blue and red portions represent the electrochemical and COLEX processes, respectively.

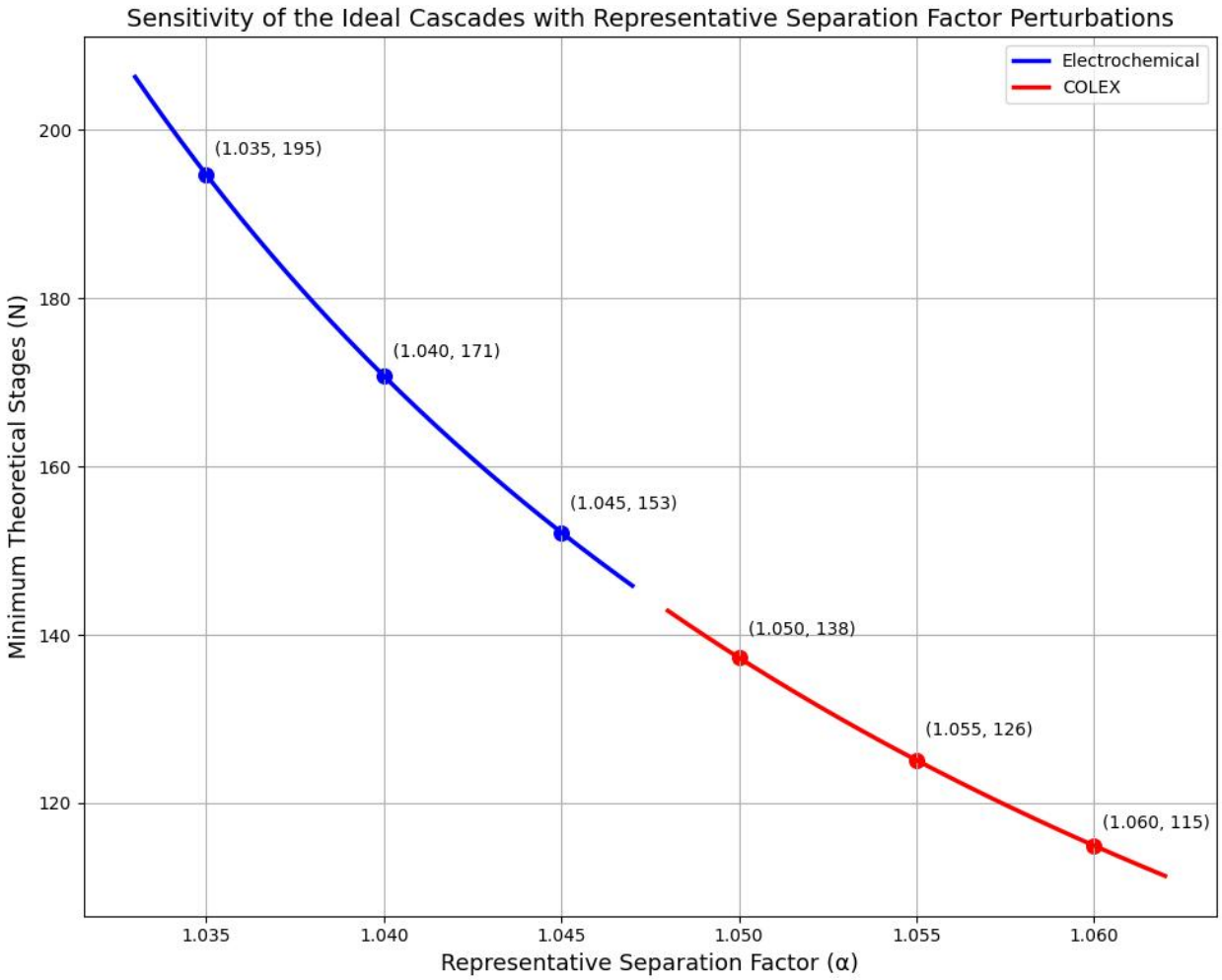

Figure 7. Sensitivity response as the minimum theoretical stage requirements for the perturbations of the representative separation factors for electrochemical and COLEX processes

Process	Representative separation factor (α)	Predicted minimum required stages (N)	Variation from baseline stage requirement	Variation in stage requirement due to change in representative separation factor (α)
Electrochemical	1.035	195	+24	More 24 stages

				required to be added to achieve 99.99% enrichment
	1.040	171	0	--
	1.045	153	-18	18 stages are needed to be reduced
COLEX	1.050	138	+12	More 12 stages required to be added to achieve 99.99% enrichment
	1.055	126	0	--
	1.060	115	-11	11 stages are needed to be eliminated

Table 3. Comparison of predicted theoretical stage requirements under variations in the representative separation factor.

Figure 7 and Table 3 present the predicted theoretical stage requirement as the response of sensitivity for the perturbation in representative separation factor. In these sensitivity responses, the electrochemical process with representative separation factor of 1.040 reached 99.99% enrichment through the 171 ideal separation stages, while with the decreased representative separation factor of 1.035, it required more 24 stages with the total of 195 theoretical stages, and with the increased representative separation factor of 1.045, it required a total of 153 theoretical stages which was decreased by 18 theoretical stages for 99.99% enrichment in ^{7}Li isotope.

In contrast, with representative separation factor of 1.055, the COLEX process required 126 theoretical stages for enriching ^{7}Li isotope natural composition (92.5%) to 99.99%. However, when the representative separation factor decreased from 1.055 to 1.050 due to unfavorable operating conditions, an additional 12 theoretical stages were required with a total of 138 to reach 99.99% enrichment in ^{7}Li. On the other hand, for the COLEX process, when the separation factor was increased from 1.055 to 1.060, the required

theoretical stages were decreased by 11 with a total of 115 for the enrichment of 99.99% ^{7}Li.

From the simulation graph in Figure 7 and data presented in Table 3, it is also observed that for decreasing the separation factor (α) ($for\ electrochemical,\ 1.040 \rightarrow 1.035;\ and\ for\ COLEX,\ 1.055 \rightarrow 1.050$) by 0.005, the required number of theoretical stages (N) increased, for the electrochemical process by 24, and for the COLEX process by 12 as sensitivity response. This implies that for decreasing the representative separation factor by 0.005, the electrochemical process is substantially more sensitive than the COLEX process (because, 24 is twice 12).

Conversely, for increasing the separation factor (α) ($for\ electrochemical,\ 1.040 \rightarrow 1.045;\ and\ for\ COLEX,\ 1.055 \rightarrow 1.060$) by 0.005, the required number of theoretical stages (N) decreased, for the electrochemical process by 18, and for the COLEX process by 11 as sensitivity response. This indicates that, for increasing the representative separation factor by 0.005, the electrochemical process is considerably more sensitive than COLEX process (because, 18 is greater than 11).

Moreover, for the overall changes of representative separation factor (α) by 0.01 (because, 1.045 - 1.035 = 0.01) for the electrochemical process, the required number of theoretical stages were changed (N) by 42 (since, 195 - 153 = 42), while for the overall changes in separation factor (α) by 0.01 (because, 1.060 - 1.050 = 0.01) for the COLEX process, the required number of theoretical stages were altered by 23 (since, 138 - 115 = 23). The overall variation for representative separation factor for both processes leads to significant changes in number of theoretical stages. This also indicated that electrochemical process is substantially more sensitive than COLEX process (because, 42 is greater than 23).

The computational predictions indicate that the electrochemical process exhibits greater sensitivity response to variations in the representative separation factor than the COLEX process. Small decreases in the representative separation factor substantially increase the theoretical stage requirements, whereas corresponding increases reduce the number of required stages. This behavior reflects the effect of comparatively lower representative separation factor adopted for the electrochemical process, where incremental changes in isotopic separation efficiency have a larger cumulative effect on the total cascade stage requirement.

On the other hand, the COLEX process demonstrates comparatively lower sensitivity because of its higher representative separation factor. Moderate variation in the representative separation factor results in relatively smaller

changes in the overall stage requirement, since each theoretical stage provides greater isotopic enrichment. Consequently, the COLEX process exhibits greater computational stability with respect to representative separation factor variations, indicating a more stable theoretical cascade requirement under the selected operating conditions.

From the practical perspective, the sensitivity analysis highlights the importance of maintaining the representative separation factor close to their selected values during process evaluation and optimization. Although both processes are affected by variations in the representative separation factor, the electrochemical process requires comparatively stricter control to minimize increases in theoretical stage requirement, whereas the COLEX process maintains relatively stable cascade characteristics over the representative range investigated in the study.

Conditional Alternative Graph for Reproducibility

In our sensitivity analysis, to facilitate the reproducibility, the computational code presents the sensitivity response of both electrochemical and COLEX processes with the executed simulation graph combinedly, when the absolute value of the difference of the representative separation factors between electrochemical and COLEX process satisfy this condition, $|\Delta\alpha| \geq 0.015$. On the other hand, if the condition $|\Delta\alpha| \geq 0.015$ is broken for choosing representative separation values of both processes, the graph will be appeared as separately to avoid the overlapping the common points.

In the present computational framework, the representative separation factors were adopted as $\alpha_{Electrochemical} = 1.040$ and $\alpha_{COLEX} = 1.055$, giving a difference of $\Delta\alpha = 0.015$ that satisfies the condition $|\Delta\alpha| \geq 0.015$; therefore, the sensitivity responses of the two processes are presented together in Figure 7.

Since our computational framework is reproducible for alternative representative separation factors, we adopted, $\alpha_{Electrochemical} = 1.040$ and $\alpha_{COLEX} = 1.050$ that breaks the condition, $|\Delta\alpha| \geq 0.015$;

because, $|\Delta\alpha| = |\alpha_{Electrochemical} - \alpha_{COLEX}| = |1.040 - 1.05| = 0.010 < 0.015$

(breaks the condition).

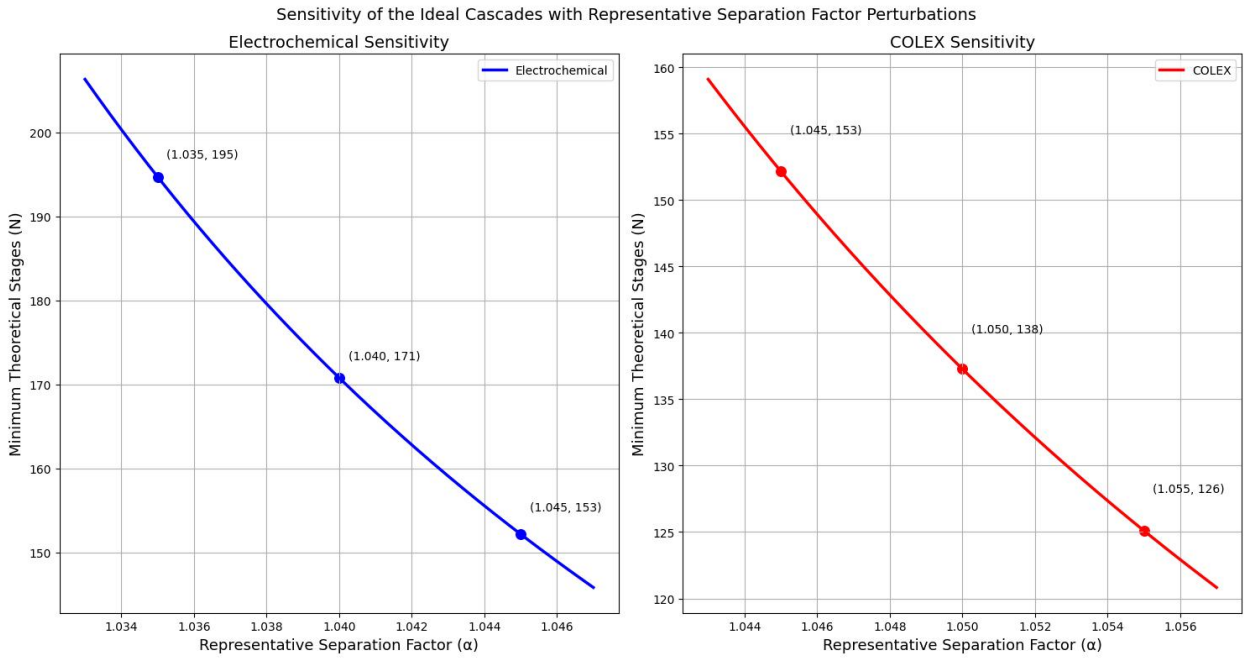

Figure 7.1. Conditional alternative graph for reproducibility, showing the sensitivity response for $\alpha_{Electrochemical} = 1.040$, $\alpha_{COLEX} = 1.050$, where $|\Delta\alpha| = 0.010 < 0.015$, presented separately for both the electrochemical and COLEX processes.

For breaking the condition, the sensitivity ranges of the two processes overlap at $\alpha = 1.045$, where both process required 153 theoretical stages. To avoid the overlapping and maintain clear comparative visualization of the point (1.045, 153) for both electrochemical and COLEX processes, the simulation graph presents the results separately in Figure 7.1. The computational code is also reproducible when $\alpha_{Electrochemical} > \alpha_{COLEX}$.

The sensitivity analysis demonstrates the dependence of the theoretical stage requirement on the representative separation factor adopted in the computational model. Based on these representative stage requirements, the subsequent section presents the operational performance prediction corresponding to the electrochemical and COLEX separation processes.

7. Enrichment Performance Predictions

The designed lithium isotope separation cascades were further evaluated to assess their enrichment performance under variations in separation

characteristics and after implementation of the adopted integer-stage allocation. Accordingly, two complementary computational analyses were conducted. First, the operational enrichment performance of the fixed cascade configurations was evaluated under unfavorable operating conditions by varying the representative separation factor. Second, the actual ^{7}Li enrichment achieved at the outlet boundaries of the individual columns was predicted using the adopted integer stage distribution. These analyses provide complementary assessments of cascade performance by considering both the influence of operational variations on a fixed cascade and the actual enrichment resulting from the designed stage allocation.

7.1 Operational Enrichment Performance Predictions of the Designed Cascades

Operational enrichment performance prediction was conducted to evaluate the influence of computational perturbations in the representative separation factor due to unfavorable operating conditions in a fixed cascade of lithium isotope separation on the enrichment performance of a fixed multicolumn cascade for the electrochemical and COLEX process. Unlike the previous sensitivity analysis, which examined the influence of variations in the representative separation factor on the theoretical stage requirements, the present analysis investigated how these variations influenced the final ^{7}Li enrichment while maintaining a fixed cascade configuration.

Previous studies showed that the separation factor may vary depending on operating conditions including applied voltage [20], pH [21], Li^{+} ion migration ratio [21], temperature [6], and electrolyte composition [22]. For example, Wang et al. showed that separation factor (α) is affected by pH and operating conditions such as voltage and Li+ ion migration ratio [21]. Oi et al. reported single-stage lithium-isotope separation factors of 1.016–1.044 over 5–50 °C, depending on the lithium salt solution [23]. According to Okuyama et al., increasing temperature reduced the lithium isotope separation factor from 1.085 to 1.028 for COLEX process [6]. Hagiwara and Takakura demonstrated that the eluent (electrolyte) composition influences the lithium isotope separation factor, with Li-acetate producing higher α values than LiOH [22]. Shin-mura et al. reported that, over a temperature range of 298.15-323.15 Kelvin, the normalized lithium isotope transfer ratio which corresponds to separation factor for electrochemical process decreased from 1.082 to 1.025 [24].

Based on these literature reports, the representative separation factors can vary with operating conditions and may be decreased under unfavorable

operating conditions. Therefore, to evaluate the operational enrichment response of the fixed cascade, two computational scenarios were introduced by reducing the representative separation factor by 0.017 and 0.009 for both processes. These equal reductions were applied to the respective representative separation factors, giving two decreased values 1.023 (because,1.040 – 0.017 = 1.023) and 1.031 (since, 1.040 – 0.009 = 1.031) for the electrochemical process and 1.038 (because, 1.055 – 0.017 = 1.038) and 1.046 (since, 1.055 – 0.009 = 1.046) for the COLEX, respectively. The selected reductions were used as computational perturbations to examine the response of final enrichment to reduced representative separation factor; they do not imply that these exact reductions in separation factor occurred under actual operating conditions. The literature reported ranges are used only to establish that separation-factor variation under unfavorable operating conditions is physically plausible.

All of the calculations were performed based on theoretical stage-enrichment relation with computational simulation using equation (7) and (8) that are derived in section 4.1, and the results are presented in Figure 8 and table 4; the corresponding code is provided in **Supplementary code LHR1** in Section 10.

For direct calculation, the minimum required ideal stage equation (9), derived in Section 4.1, can be rearranged as follows

$$N = \frac{ln\{\frac{x_p(1-x_f)}{x_f(1-x_p)}\}}{ln(\alpha)}$$

$$\Rightarrow\ x_p = \frac{x_f\alpha^N}{1 - x_f + x_f\alpha^N} \text{ .....(10)}$$

This expression can be used for direct calculation. For example: when $\alpha = 1.023$, $x_f = 0.925$, and N = 171,

$$\therefore enrichment, x_p = \frac{x_f\alpha^N}{1 - x_f + x_f\alpha^N} = \frac{0.925\times1.023^{171}}{1-0.925+0.925 \times 1.023^{171}} = 0.99834 = 99.834\%$$

In the computational simulation, to calculate the predicted final enrichment (x_p) for each selected representative separation factor of electrochemical and COLEX processes, a simulation graph was generated by plotting the

representative separation factor (α) against the predicted final ^{7}Li enrichment (x_p) for both the electrochemical and COLEX processes.

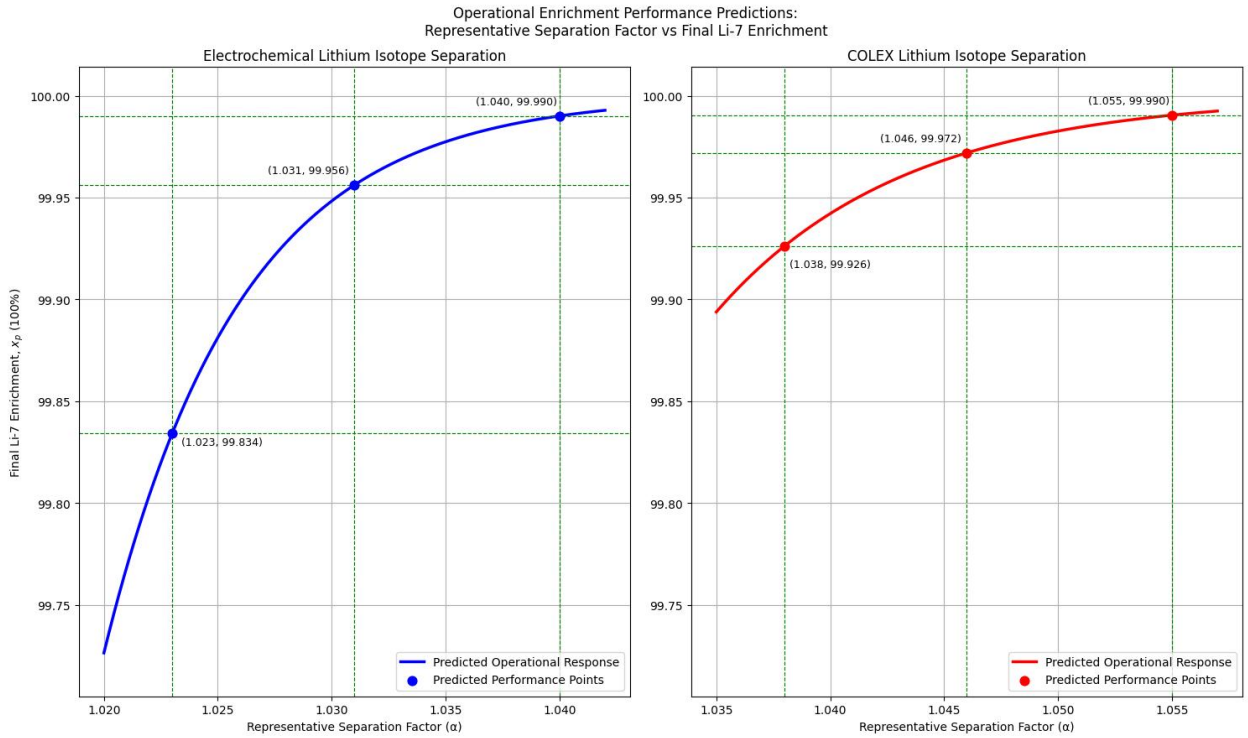

Figure 8. Operational performance of the fixed cascade configuration under variations in the representative separation factor for electrochemical and COLEX lithium isotope separation processes.

Process	Representative separation factor (α)	Predicted Li-7 enrichment (%)	Variation from target enrichment (percentage points)	Operational Interpretation
Electrochemical	1.023	99.834	0.156	Reduced enrichment
	1.031	99.956	0.034	Improved, but still away from target enrichment
	1.040	99.990	0.000	Target enrichment

				achieved
COLEX	1.038	99.926	0.064	Reduced enrichment
	1.046	99.972	0.018	Improved, but still away from target enrichment
	1.055	99.990	0.000	Target enrichment achieved

Table 4. Predicted final ^{7}Li enrichment of the fixed cascade under variations in the representative separation factor for the electrochemical and COLEX processes.

The simulation results, presented in Figure 8 and table 4, show that for the fixed electrochemical cascade, a representative separation factor of 1.040 achieves the target 99.99% enrichment in ^{7}Li. When the separation factor was reduced to 1.023 and 1.031 under assumed unfavorable operating-condition scenarios, the simulations predicted final ^{7}Li enrichments of 99.834% and 99.956%, respectively.

Similarly, for the simulation results of the COLEX process for the fixed cascade system, for the representative separation factor of 1.055, 99.990% enrichment in ^{7}Li was achieved. When the representative separation factor decreased to 1.038 and 1.046 under unfavorable operating-condition scenarios, the computational simulation predicted 99.926% and 99.972% ^{7}Li enrichment, respectively.

For the equal reduction of 0.017 in representative separation factors at $\alpha_{Electrochemical} = 1.023$, $\alpha_{COLEX} = 1.038$, the electrochemical process showed a 0.156 percentage-points reduction in final ^{7}Li enrichment , whereas the corresponding reduction for COLEX process was only 0.064 percentage points. Similarly, for the equal reduction 0.009 in the representative separation factors at $\alpha_{Electrochemical} = 1.031$, $\alpha_{COLEX} = 1.046$, the electrochemical process exhibited a 0.034 percentage-point reduction, compared with 0.018 percentage-point reduction for the COLEX. Since 0.156 is greater than 0.064, and 0.034 is greater than 0.018, the computational simulation results indicate that the electrochemical process exhibited a greater reduction in final enrichment under the evaluated operational enrichment variations than the COLEX process. These results also indicate that COLEX process exhibits greater operational stability than electrochemical process under the evaluated representative separation factor reductions.

The present operational performance prediction highlights the importance of maintaining stable operational conditions in lithium isotope separation systems. The operational performance analysis demonstrates that the computational model can predict the influence of the specified variation in the representative separation factor on lithium isotope enrichment with a fixed cascade configuration. The computational simulation indicates that even relatively small reduction in the representative separation factor may reduce the final ^{7}Li enrichment achieved with a fixed cascade configuration. Therefore, careful monitoring and control of these operational conditions are essential for maintaining the desired enrichment performance in practical applications.

7.2 Column-Wise Actual Enrichment After Rounded Stage Allocation

Based on the three nominal incremental enrichment sections, the cascade stage distribution was established in the range of 92.5–95%, 95–99%, and 99–99.99% ^{7}Li enrichments (details in Section 5). However, the first two column stage requirements were rounded upward, while the final column was assigned the residual number of stages required to preserve the previously established total of cascade stage count. Consequently, the actual enrichment achieved at the outlet of each column may differ from the nominal enrichment boundaries used for the incremental stage allocation. Therefore, the actual ^{7}Li enrichment corresponding to the adopted integer stage distribution was predicted at each column boundary to assess the enrichment achieved by the designed cascade.

A computational simulation was developed based on theoretical stage-enrichment relationship using Equations (7) and (8) derived in Section 4.1 to determine the actual ^{7}Li enrichment corresponding to the adopted integer stage allocation for each column. The calculations were performed using computational simulation and the results are presented in Figure 9, 10 and table 5; the corresponding code is provided in **Supplementary code LHR1** in Section 10.

For direct calculation Equation (10) can be used. For example: In column-1 of electrochemical process $\alpha = 1.040,\ x_f = 0.925,$ and $\mathrm{N} = 171,$

actual enrichment in column-1, $x_p = \frac{x_f \alpha^N}{1 - x_f + x_f \alpha^N}$

$$= \frac{0.925 \times 1.040^{12}}{1 - 0.925 + 0.925 \times 1.040^{12}} = 0.95179809 = 95.179809\%$$

The computational simulation evaluated the ^{7}Li enrichment (x_p) as a function of the cumulative number of theoretical stages (N) for the representative separation factor of each process. The resulting N-x_p relationship was plotted to identify the actual enrichment at the cumulative stage positions corresponding to the boundaries of column-1, column-2 and column-3.

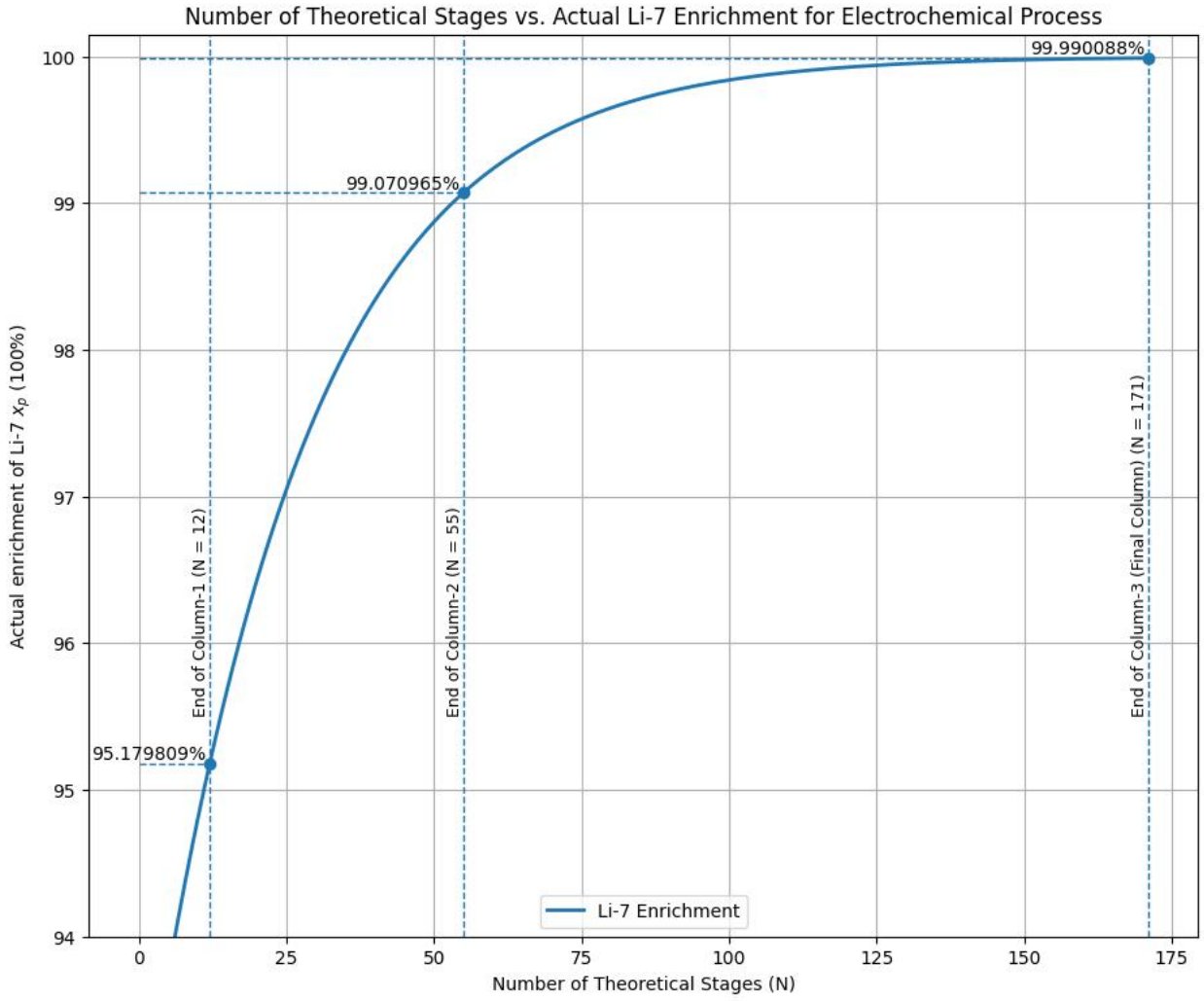

Figure 9. Actual ^{7}Li enrichment as a function of the number of theoretical stages for the electrochemical process, showing the enrichment at the

cumulative stage positions corresponding to the outlet boundaries of column-1, column-2 and column-3.

For the electrochemical process, column-1 contains 12 theoretical stages, while column-2 contains 55 -12 = 43 stages, corresponding to cumulative stage positions of N = 12 and N = 55, respectively. The remaining 171− 55 = 116 stages are allocated to Column 3, giving the final cumulative stage position of N = 171. Similarly, for the COLEX process, column-1 contains 9 theoretical stages, column-2 contains 40−9=31 stages, and column-3 contains 126−40=86 stages, corresponding to cumulative stage positions of N = 9, N = 40, and N = 126, respectively (details in Section 5).

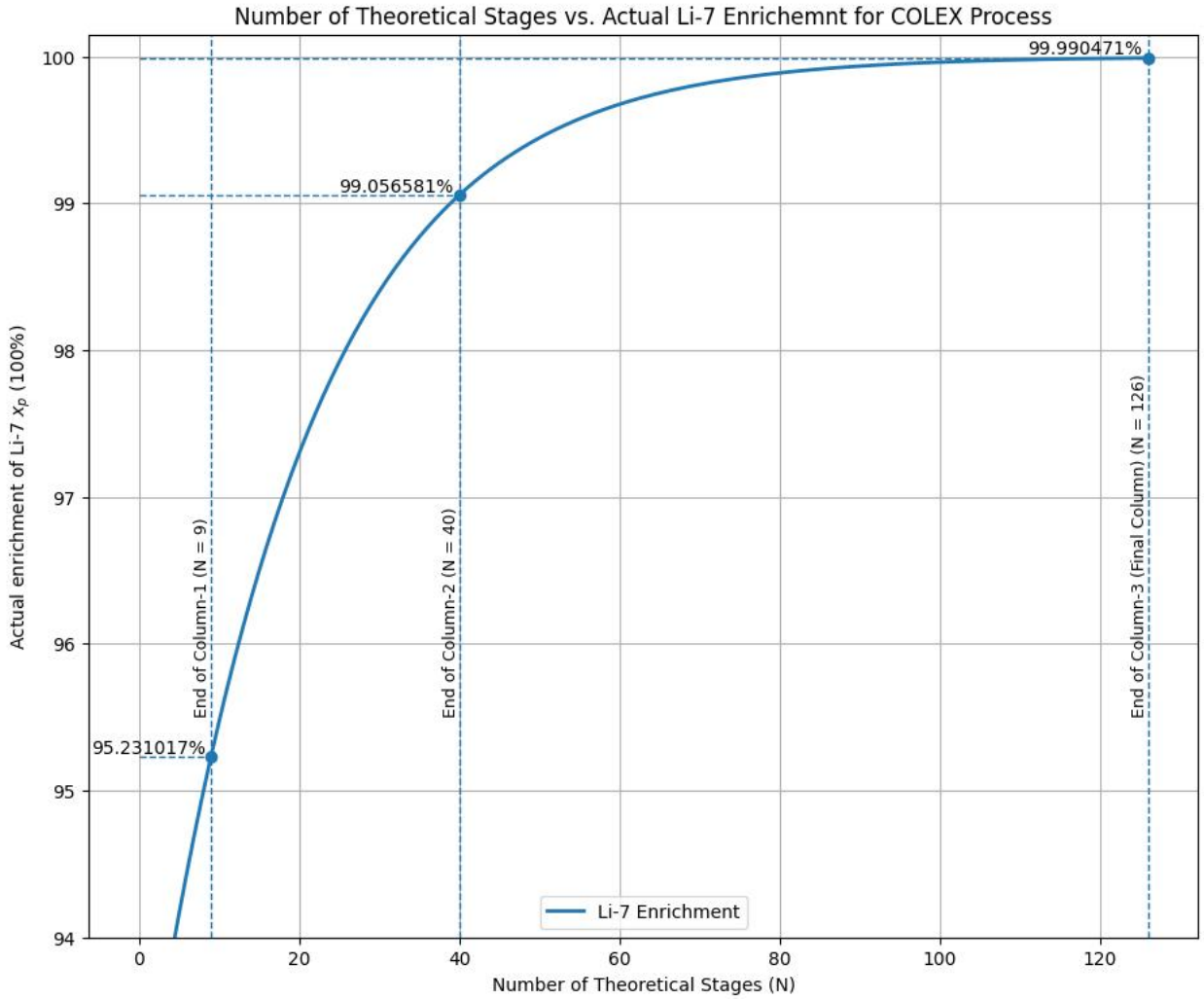

Figure 10. Actual ^{7}Li enrichment as a function of the number of theoretical stages for the COLEX process, showing the enrichment at the cumulative stage

positions corresponding to the outlet boundaries of column-1, column-2 and column-3.

Cascade Boundary	Nominal enrichment boundary (%)	Electrochemical actual enrichment (%)	COlEX actual enrichment (%)	COLEX - Electrochemical (percentage points)	Higher actual enrichment
Column-1	95.000000	95.179809	95.231017	+0.051208	COLEX
Column-2	99.000000	99.070965	99.056581	-0.014384	Electrochemical
Column-3	99.990000	99.990088	99.990471	+0.000383	COLEX

Table 5. Comparison of nominal and actual 7Li enrichment at the outlet boundaries of column-1, column-2 and column-3 for the electrochemical and COLEX cascades.

For the electrochemical process, the computational simulation results presented in Figure 9 and Table 5, the cascade started to enrich ^{7}Li with a natural ^{7}Li composition of 92.500%. The 12 theoretical stages allocated to column-1 increased the ^{7}Li enrichment from 92.500% to 95.179809%. Column-2, containing an additional 43 theoretical stages and therefore reaching the cumulative stage position N = 55, further increased the enrichment from 95.179809% to 99.070965%. Finally, the 116 stages allocated to column-3 increased the enrichment from 99.070965% to 99.990088% at the cumulative stage position N = 171. Thus, the electrochemical cascade, with rounded 171 stages, achieved an overall 99.990088% ^{7}Li enrichment that slightly above the target value of 99.99%.

Similarly, in the COLEX process, it is observed from the Figure 10 and Table 5 that the column-1, containing 9 theoretical stages, enriched ^{7}Li from 92.500% to 95.231017%. The subsequent 31 stages in column-2, corresponding to the cumulative stage position N = 40, increased the enrichment further to 99.056581%. The remaining 86 stages in column-3, then, increased the enrichment to 99.990471% at the final cumulative stage position N = 126. Thus, the COLEX process with rounded 126 stages achieved an overall ^{7}Li enrichment of 99.990471% that is slightly above the target value of 99.99%.

Comparison with the nominal enrichment boundaries shows that the actual column-wise enrichments deviate slightly from the nominal values used to define the incremental enrichment sections. For the electrochemical process, the actual enrichment at the end of column-1 (95.179809%) is 0.179809 percentage points higher than the nominal boundary of 95%, while the enrichment at the end of column-2 (99.070965%) is 0.070965 percentage points higher than the nominal 99% boundary. The final enrichment of 99.990088% is also slightly higher than the nominal target of 99.99%, by 0.000088 percentage points. For the COLEX process, the corresponding deviations are 0.231017 percentage points above the 95% boundary at the end of column-1, 0.056581 percentage points above the 99% boundary at the end of column-2, and 0.000471 percentage points above the 99.99% target at the final cascade outlet. These deviations arise from the adoption of integer stage numbers and the resulting cumulative stage positions, rather than from a change in the nominal enrichment boundaries used for the initial cascade design.

A comparison between the two processes (presented in table 5) shows that COLEX provides higher actual enrichment in ^{7}Li at the column-1 boundary, whereas the electrochemical process provides slightly higher enrichment at the column-2 boundary. Specifically, column-1 reaches 95.231017% for COLEX compared with 95.179809% for the electrochemical process, giving COLEX an enrichment advantage of 0.051208 percentage points. At the column-2 boundary, however, the electrochemical process reaches 99.070965%, compared with 99.056581% for COLEX, giving the electrochemical process an advantage of 0.014384 percentage points. At the final cascade boundary, both processes achieve enrichment above the 99.99% target, with COLEX reaching 99.990471% and the electrochemical process reaching 99.990088%; thus, COLEX provides a marginally higher final enrichment by 0.000383 percentage points. Overall, the difference between the two processes is very small at the final cascade outlet, despite their different representative separation factors and stage requirements.

Overall, the column-wise enrichment prediction demonstrates that the integer stage allocation produces actual enrichment profiles that differ slightly from the nominal incremental enrichment boundaries used in the cascade design. Both processes nevertheless achieve ^{7}Li enrichment above the 99.99% target at their respective final cascade boundaries, with 99.990088% for the electrochemical process and 99.990471% for the COLEX process. The comparison further shows that COLEX provides slightly higher enrichment at the column-1 and column-3 boundaries, whereas the electrochemical process

gives marginally higher enrichment at the column-2 boundary. These small differences arise from the combined effects of the representative separation factors and the different integer stage allocations of the two cascades. The predicted column-wise enrichments therefore provide a direct quantitative verification of the enrichment actually achieved by the designed integer-stage cascades and complement the nominal incremental enrichment framework used for cascade configuration.

Finally, the computational analyses demonstrate that the designed lithium isotope separation cascades can be evaluated from both operational and stage-allocation perspectives. The operational performance analysis showed that reductions in the representative separation factor under the evaluated unfavorable operating conditions reduce the final ^{7}Li enrichment of the fixed cascades, with the electrochemical process exhibiting a greater enrichment response than the COLEX process to the evaluated separation-factor perturbations. In contrast, the column-wise actual-enrichment analysis showed that the adopted integer-stage allocations resulted in enrichment values slightly different from the nominal incremental boundaries, while both cascades achieved ^{7}Li enrichment above the 99.99% target at their final outlets. Together, these results demonstrate the applicability of the developed computational procedure for evaluating both the operational response and the actual enrichment performance of the designed multicolumn cascades.

8. Results and Discussion

The theoretical predicted results are obtained from computational simulation framework for electrochemical and COLEX processes. The results are integrated here to evaluate theoretical stage requirements, cascade configurations, sensitivity response for variation in representative separation factors, operational enrichment performances prediction, and column-wise actual enrichment under ideal model assumptions.

Parameter	Electrochemical Process	COLEX Process	Comparative Comment
Selected Representative separation factor (α)	1.040	1.055	Selected from reported values
Target ^{7}Li enrichment	99.99%	99.99%	Same enrichment target for both

			processes
Theoretical stage requirement	171 stages	126 stages	COLEX process requires fewer theoretical stages
Theoretical stage distribution among column-1, column-2 and column-3	12, 43, 116 stages respectively	9, 31, 86 stages respectively	Each column of electrochemical contains greater number of stages than COLEX
Variation in sensitivity to variation in separation factor	Higher	Lower	Electrochemical process is more sensitive than COLEX
Cascade configuration	Larger conceptual cascade	More compact conceptual cascade	Higher representative separation factor reduces theoretical cascade complexity for COLEX process
Operational enrichment with $\alpha_{Electrochemical} = 1.023, and\ \alpha_{COLEX} = 1.031$	99.834% and 99.956%, respectively	99.926% and 99.972%, respectively	
With reduction ranges of 0.017 and 0.009 in representative separation factor, the enrichments reduced by	0.156 and 0.034 percentage points respectively compared with 99.99% target enrichment.	0.064 and 0.018 percentage points, respectively compared with 99.99% target enrichment.	Greater enrichment reduction in electrochemical process than COLEX process
Actual enrichment in column-1, column-2, and column-3	95.179809%, 99.070965%, and 99.990088% respectively	95.231017%, 99.056581%, and 99.990471% respectively	COLEX exhibits higher enrichment in column-1 and 3; while electrochemical shows higher enrichment in column-2
Computational relation of representative separation factor (α) with total required stages	Smaller representative separation factor (1.040) corresponds to higher theoretical stage requirement (171)	Higher representative separation factor (1.055) corresponds to lower	N decreases as α increases

(N)		theoretical stage requirement (126)	

Table 6. Integrated comparative assessment of the electrochemical and COLEX lithium isotope separation processes based on the computational predictions of the present study.

The integrated computational predictions for both processes are comparatively presented in Table 6. These results reveal that the relative computational performance of the electrochemical and COLEX processes depends on cascade configuration and enrichment performance under adopted assumptions. The results of the study demonstrate the following -

1. With representative separation factor 1.040, the electrochemical process required a minimum of 171 theoretical stages; whereas with representative separation factor 1.055, the COLEX process required a minimum of 126 theoretical stages to reach nominal 99.99% ^{7}Li enrichment.

2. With the representative separation factor 1.040, the minimum required theoretical stages of 171 for electrochemical process were distributed among three cascade columns: column-1, column-2 and column-3 with 12, 43 and 116, respectively. Similarly, with representative separation factor 1.055, for the COLEX process the minimum theoretical stage requirement of 126 were distributed among column-1, column-2 and column-3 as 9, 31 and 86, respectively.

3. In sensitivity analysis for perturbed in representative separation factor (α), the electrochemical process required 195 stages at $\alpha = 1.035$ and 153 stages at $\alpha = 1.045$, while the COLEX process required 138 stages at $\alpha = 1.050$, and 115 stages at $\alpha = 1.060$, relative to their representative values of 1.040 and 1.055, respectively. With perturbation in representative separation factor, in the range of 0.005 above the representative separation factor, below the representative separation factor, or even in the whole range of 0.01, electrochemical process showed substantially more sensitivity than COLEX process. This demonstrates that COLEX process is more stable than electrochemical process indicating that electrochemical process requires stricter operational control. From a

theoretical perspective, the higher sensitivity is consistent with the comparatively lower representative separation factor of the electrochemical process, where small changes in isotopic representative separation factor lead to larger changes in the total theoretical stage requirement over the entire cascade.

4. In operational enrichment performance predictions in electrochemical process, with equal decrease in representative separation factor of 0.017 and 0.009 for both processes, the electrochemical process 99.834%, 99.956% ^{7}Li enrichment were predicted and exhibited enrichment reductions of 0.156 and 0.034 percentage points, respectively; whereas the corresponding ^{7}Li enrichment values for the COLEX process are 99.926% and 99.972%, and the reductions were only 0.064 and 0.018 percentage points, respectively compared with target enrichment 99.990%. These results (0.156 is greater than 0.064, and 0.034 is greater than 0.018) indicate that the electrochemical process is more susceptible to operational perturbations and therefore requires stricter operational control than the COLEX process.

5. In column-wise actual enrichment prediction for column-1, column-2 and column-3, electrochemical process demonstrated 95.179809%, 99.070965%, and 99.990088%; while COLEX process exhibited 95.231017%, 99.056581%, and 99.990471% respectively. The COLEX process showed enrichment variation 0.051208 in column-1, and 0.000383 in column-3; whereas electrochemical process exhibited enrichment variation 0.014384 in column-2. These prediction results indicate COLEX exhibits higher enrichment in column-1 and column-3; while electrochemical shows higher enrichment in column-2.

Overall, the computational simulation results indicate that COLEX achieves small number of theoretical stages, a more compact cascade configuration, lower sensitivity to representative separation factor variation, and smaller enrichment deviation predictions under the adopted conditions, primarily because of its higher representative separation factor. In contrast, electrochemical process requires a larger theoretical cascade, higher sensitivity and greater enrichment reduction as its representative separation factor smaller than that of COLEX. Thus, the computational framework enables process-level comparative presentation by integrating stage requirement, cascade configuration, sensitivity analysis, enrichment performance, and column-wise actual enrichment under consistent modeling assumptions.

When two processes are evaluated simultaneously using the master code of integrated computational framework, their predicted cascade configuration and enrichment performances can be compared consistently. This parameterized structure enables the framework to be reproduced and extended for alternative feed composition (x_f), production composition or target enrichment (x_p), and the respective representative separation factors (α) without reformulating the underlying computational framework. Since, intermediate ^{7}Li enrichment of 95% and 99% were our nominal boundary, the framework is conditioned to $x_f < 0.95, and\ x_p > 0.99$ for a valid cascade configuration and enrichment performance according to our computational framework. Although the target enrichment of the present study is 99.99% ^{7}Li, our computational framework can predict above or below of 99.99% ^{7}Li target enrichment changing the target value of x_p.

A limitation of the present operational enrichment performance prediction (Section 7.1) prediction is that the decreased representative separation factors due to unfavorable condition are introduced as assumed computational scenarios rather than being obtained from direct experimental report or derived from a process specific model of operating-condition changes. The literature reported values were used to support the selected alternative decreased values may correspond to different process and operating conditions. Furthermore, the simultaneous effects of multiple process and operating parameters on separation performance are not explicitly resolved. Consequently, the resulting enrichment deviations should be interpreted as scenario-based computational predictions rather than experimentally observed operational changes. Future work incorporating coupled process-condition effects and experimental validation would improve the physical basis of operational enrichment performance prediction.

9. Conclusion

The present study develops a reproducible computational framework for predicting minimum theoretical stage requirements, multicolumn cascade configurations and stage distributions, sensitivity response to representative separation-factor variation, and enrichment performance for lithium isotope separation. The framework was demonstrated using electrochemical and COLEX processes under identical ideal counter-current multistage-cascade assumptions for a target ^{7}Li enrichment of 99.99%. A representative separation factor was assigned to each process as the principal process-specific input along with feed composition and target enrichment, enabling the computational

procedure to be applied consistently and reproduced for alternative input conditions.

The computational framework predicted 171 theoretical stages for the electrochemical process and 126 stages for COLEX at representative separation factors of 1.040 and 1.055, respectively. The corresponding three-column cascade distributions were 12, 43 and 116 stages for electrochemical process and 9, 31 and 86 stages for COLEX. Sensitivity analysis demonstrated that the electrochemical process was more sensitive to representative separation-factor variation than COLEX, while the operational enrichment performance scenarios showed larger predicted enrichment reductions for electrochemical separation under the respective assumed unfavorable reductions to decrease in representative separation factor. Column-wise analysis further demonstrated the actual enrichment progression through the designed cascade configurations.

The column-wise actual enrichment performance after rounded stage allocation further confirmed the performance of the designed cascades. Slight deviations from the nominal enrichment boundaries occurred because of integer stage allocation and total integer stage determination for the cascades. Both processes achieved slightly above 99.99% ^{7}Li enrichment. COLEX process exhibited slightly higher enrichment at the outlets of column-1 and column-3, whereas electrochemical process showed slightly higher enrichment at column-2, demonstrating distinct column-wise enrichment behavior between the two processes.

The reproducibility of the computational framework arises from its parameterized implementation, through which feed composition (x_f), target enrichment (x_p), and representative separation factors (α) can be varied to regenerate the outputs without reformulating the underlying procedure while retaining the nominal intermediate column enrichment boundaries of 95% and 99%. The framework can therefore be applied to evaluate multiple processes simultaneously under a common computational basis, even beyond the 99.99% ^{7}Li target enrichment. The comparative presentation of electrochemical and COLEX processes demonstrates this applicability while providing a consistent computational basis for interpreting differences in stage requirements, cascade configuration, sensitivity, and enrichment performance.

The operational enrichment performance prediction introduces reductions in representative separation factors as unfavorable scenarios in our computational study, while literature-reported separation factor values and ranges provide supporting context for the selected alternative values. These scenarios should therefore be interpreted as computational predictions rather than experimentally observed operational changes. The framework does not

explicitly resolve the simultaneous effects of multiple process and operating parameters, detailed transport phenomena, energy consumption, or economic considerations. Future work incorporating coupled process-condition effects, realistic stage behavior, energy and economic assessment, and experimental validation can extend the framework toward more detailed process modeling and engineering application.

10. Supplementary Code and Data

The computational code used to generate the results reported in this study provided as **Supplementary Code LHR1** in the form of an executable Google Colab Notebook. The link is as follows:

https://colab.research.google.com/drive/14WOEHyGd1qZTltpogKv0vNF1pnLnXblz?usp=sharing

Cell 1: Section 4.2 – Code for Figure 4

Cell 2: Section 5 – Code for Figure 5

Cell 3: Section 5 – Code for Figure 6

Cell 4: Section 6 – Code for Figure 7 or 7.1

Cell 5: Section 7.1 – Code for figure 8

Cell 6: Section 7.2 – Code for Figure 9

Cell 7: Section 7.2 – Code for Figure 10

Cell 8: Master Code for Integrated Computational Framework

Reproducibility Test Results of the Master Code for Integrated Computational Framework:

In the reproducibility test, four tests are performed using different combinations of feed composition (x_f), target enrichment (x_p), representative separation factors of electrochemical ($\alpha_{Electrochemical}$) and COLEX (α_{COLEX}) processes with the Master Code for Integrated Computational Framework, and the results are presented below gradually.

Reproducibility Test 1: (Baseline test)

When, $\alpha_{Electrochemical} = 1.040,\ \alpha_{COLEX} = 1.055,\ x_f = 0.925,\ and\ x_p = 0.9999;$

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======================================================================
SECTION 4.2 — DETERMINATION OF MINIMUM THEORETICAL STAGE REQUIREMENTS FOR
ELECTROCHEMICAL AND COLEX PROCESSES
======================================================================
```

	Process	Feed fraction xf	Target product fraction xp	Representative alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	0.92500	0.999900	1.040	170.775	171
1	COLEX	0.92500	0.999900	1.055	125.100	126

```
======================================================================
SECTION 5 — CASCADE CONFIGURATION AND STAGE DISTRIBUTION
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Representative separation factor	1.04	1.055
1	Column 1: 92.500000% → 95.000000%	12.00	9.000
2	Column 2: 95.000000% → 99.000000%	43.00	31.000
3	Column 3: 99.000000% → 99.990000%	116.00	86.000
4	Total theoretical stages	171.00	126.000

```
CASCADE CALCULATION DETAILS
----------------------------------------------------------------------
```

	Parameter	Electrochemical	COLEX
0	Overall continuous stage requirement	170.775445	125.099716
1	Overall minimum integer stages N	171.000000	126.000000
2	Column 1 continuous requirement	11.017988	8.071109
3	Column 1 integer stages N1	12.000000	9.000000
4	Column 2 continuous requirement	42.086967	30.830355

	Parameter	Electrochemical	COLEX
5	Column 2 integer stages N2	43.000000	31.000000
6	Column 3 continuous requirement	117.670490	86.198252
7	Column 3 allocated stages N3	116.000000	86.000000
8	Total allocated stages	171.000000	126.000000

==========
SECTION 6 — SENSITIVITY ANALYSIS OF THE IDEAL CASCADES WITH REPRESENTATIVE SEPARATION FACTOR PERTURBATIONS
==========

	Process	Representative alpha	Sensitivity alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	1.040	1.035	194.699	195
1	Electrochemical	1.040	1.040	170.775	171
2	Electrochemical	1.040	1.045	152.167	153
3	COLEX	1.055	1.050	137.280	138
4	COLEX	1.055	1.055	125.100	126
5	COLEX	1.055	1.060	114.949	115

==========
SECTION 7.1 — OPERATIONAL ENRICHMENT PERFORMANCE PREDICTIONS OF THE DESIGNED CASCADES
==========

	Process	Designed stages N	Representative alpha	Evaluated alpha	Predicted final Li-7 enrichment (%)
0	Electrochemical	171	1.040	1.023	99.834245
1	Electrochemical	171	1.040	1.031	99.956198

	Process	Designed stages N	Representative alpha	Evaluated alpha	Predicted final Li-7 enrichment (%)
2	Electrochemical	171	1.040	1.040	99.990088
3	COLEX	126	1.055	1.038	99.926255
4	COLEX	126	1.055	1.046	99.971958
5	COLEX	126	1.055	1.055	99.990471

```
======================================================================
SECTION 7.2 — COLUMN-WISE ACTUAL ENRICHMENT AFTER ROUNDED STAGE ALLOCATION
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Column 1 actual Li-7 enrichment (%)	95.179809	95.231017
1	Column 2 actual Li-7 enrichment (%)	99.070965	99.056581
2	Column 3 actual Li-7 enrichment (%)	99.990088	99.990471

```
======================================================================
SEQUENTIAL CASCADE PERFORMANCE VERIFICATION
======================================================================
```

	Process	Column 1 stages	Column 2 stages	Column 3 stages	Total stages	Final Li-7 enrichment (%)
0	Electrochemical	12	43	116	171	99.990088
1	COLEX	9	31	86	126	99.990471

```
======================================================================
COMPARATIVE INTERPRETATION
======================================================================
✓ EC requires more theoretical stages than COLEX: 171 > 126
Stage difference (EC - COLEX) = 45 stages
COLEX requires approximately 26.316% fewer stages than EC.
EC sensitivity range = 42 stages
COLEX sensitivity range = 23 stages
✓ Electrochemical separation is more sensitive to the specified separation-
factor variation than COLEX.

Enrichment Performance Predictions:
✓ For the same absolute deviation range of the representative separation
factor, the electrochemical,
```

process showed a greater enrichment deviation than COLEX.
✓ These prediction results indicate COLEX exhibits higher , enrichment in Column 1 and Column 3, while the electrochemical process shows higher enrichment in Column 2.

==========
INTEGRATED REPRODUCIBLE COMPARATIVE SUMMARY
==========

	Parameter	Electrochemical	COLEX
0	Feed Li-7 fraction, xf	0.925000	0.925000
1	Target Li-7 fraction, xp	0.999900	0.999900
2	Representative separation factor, alpha	1.040000	1.055000
3	Continuous total stage requirement	170.775445	125.099716
4	Minimum theoretical stages, N	171.000000	126.000000
5	Column 1 stages	12.000000	9.000000
6	Column 2 stages	43.000000	31.000000
7	Column 3 stages	116.000000	86.000000
8	Total cascade stages	171.000000	126.000000
9	Sensitivity alpha — low	1.035000	1.050000
10	Sensitivity stages — low	195.000000	138.000000
11	Sensitivity alpha — representative	1.040000	1.055000
12	Sensitivity stages — representative	171.000000	126.000000
13	Sensitivity alpha — high	1.045000	1.060000
14	Sensitivity stages — high	153.000000	115.000000
15	Operational alpha — low	1.023000	1.038000
16	Predicted enrichment (%) — low	99.834245	99.926255
17	Operational alpha — intermediate	1.031000	1.046000
18	Predicted enrichment (%) — intermediate	99.956198	99.971958
19	Operational alpha — representative	1.040000	1.055000

	Parameter	Electrochemical	COLEX
20	Predicted enrichment (%) — representative	99.990088	99.990471
21	Column 1 actual Li-7 enrichment (%)	95.179809	95.231017
22	Column 2 actual Li-7 enrichment (%)	99.070965	99.056581
23	Column 3 actual Li-7 enrichment (%)	99.990088	99.990471
24	Sequential cascade final enrichment (%)	99.990088	99.990471

```
======================================================================
AUTOMATED CONSISTENCY CHECKS
======================================================================
✓ Baseline EC stage requirement = 171
✓ Baseline COLEX stage requirement = 126
✓ EC minimum stage requirement = 171
✓ COLEX minimum stage requirement = 126
✓ EC cascade distribution = 12 + 43 + 116 = 171
✓ COLEX cascade distribution = 9 + 31 + 86 = 126
✓ Column 1 and Column 2 ceiling operations verified
✓ Column 3 residual-stage allocation verified
✓ EC sequential cascade reaches/exceeds 99.990000% Li-7 target
✓ COLEX sequential cascade reaches/exceeds 99.990000% Li-7

ALL CONSISTENCY CHECKS PASSED.
```

Reproducibility Test 2:

When, $\alpha_{Electrochemical} = 1.045,\ \alpha_{COLEX} = 1.060,\ x_f = 0.925,\ and\ x_p = 0.99995$;

```
======================================================================
SECTION 4.2 — DETERMINATION OF MINIMUM THEORETICAL STAGE REQUIREMENTS FOR
ELECTROCHEMICAL AND COLEX PROCESSES
======================================================================
```

	Process	Feed fraction xf	Target product fraction xp	Representative alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	0.92500	0.999950	1.045	167.916	168
1	COLEX	0.92500	0.999950	1.060	126.845	127

```
======================================================================
SECTION 5 — CASCADE CONFIGURATION AND STAGE DISTRIBUTION
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Representative separation factor	1.045	1.06
1	Column 1: 92.500000% → 95.000000%	10.000	8.00
2	Column 2: 95.000000% → 99.000000%	38.000	29.00
3	Column 3: 99.000000% → 99.995000%	120.000	90.00
4	Total theoretical stages	168.000	127.00

CASCADE CALCULATION DETAILS

	Parameter	Electrochemical	COLEX
0	Overall continuous stage requirement	167.915832	126.845211
1	Overall minimum integer stages N	168.000000	127.000000
2	Column 1 continuous requirement	9.817445	7.416191
3	Column 1 integer stages N1	10.000000	8.000000
4	Column 2 continuous requirement	37.501083	28.328673
5	Column 2 integer stages N2	38.000000	29.000000
6	Column 3 continuous requirement	120.597304	91.100346
7	Column 3 allocated stages N3	120.000000	90.000000
8	Total allocated stages	168.000000	127.000000

```
======================================================================
SECTION 6 — SENSITIVITY ANALYSIS OF THE IDEAL CASCADES WITH REPRESENTATIVE
SEPARATION FACTOR PERTURBATIONS
======================================================================
```

	Process	Representative alpha	Sensitivity alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemica	1.045	1.040	188.450	189

	Process	Representative alpha	Sensitivity alpha	Continuous stage requirement	Minimum theoretical stages N
	l				
1	Electrochemical	1.045	1.045	167.916	168
2	Electrochemical	1.045	1.050	151.488	152
3	COLEX	1.060	1.055	138.047	139
4	COLEX	1.060	1.060	126.845	127
5	COLEX	1.060	1.065	117.367	118

==========
SECTION 7.1 — OPERATIONAL ENRICHMENT PERFORMANCE PREDICTIONS OF THE DESIGNED CASCADES
==========

	Process	Designed stages N	Representative alpha	Evaluated alpha	Predicted final Li-7 enrichment (%)
0	Electrochemical	168	1.045	1.028	99.921705
1	Electrochemical	168	1.045	1.036	99.978700
2	Electrochemical	168	1.045	1.045	99.995018
3	COLEX	127	1.060	1.043	99.961395
4	COLEX	127	1.060	1.051	99.985368
5	COLEX	127	1.060	1.060	99.995045

==========
SECTION 7.2 — COLUMN-WISE ACTUAL ENRICHMENT AFTER ROUNDED STAGE ALLOCATION
==========

	Parameter	Electrochemical	COLEX
0	Column 1 actual Li-7 enrichment (%)	95.038031	95.159134

	Parameter	Electrochemical	COLEX
1	Column 2 actual Li-7 enrichment (%)	99.029264	99.069869
2	Column 3 actual Li-7 enrichment (%)	99.995018	99.995045

```
======================================================================
SEQUENTIAL CASCADE PERFORMANCE VERIFICATION
======================================================================
```

	Process	Column 1 stages	Column 2 stages	Column 3 stages	Total stages	Final Li-7 enrichment (%)
0	Electrochemical	10	38	120	168	99.995018
1	COLEX	8	29	90	127	99.995045

```
======================================================================
COMPARATIVE INTERPRETATION
======================================================================
✓ EC requires more theoretical stages than COLEX: 168 > 127
Stage difference (EC - COLEX) = 41 stages
COLEX requires approximately 24.405% fewer stages than EC.
EC sensitivity range = 37 stages
COLEX sensitivity range = 21 stages
✓ Electrochemical separation is more sensitive to the specified separation-
factor variation than COLEX.

Enrichment Performance Predictions:
✓ For the same absolute deviation range of the representative separation
factor, the electrochemical,
 process showed a greater enrichment deviation than COLEX.
✓ These prediction results indicate COLEX exhibits higher enrichment in all
three columns.

======================================================================
INTEGRATED REPRODUCIBLE COMPARATIVE SUMMARY
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Feed Li-7 fraction, xf	0.925000	0.925000
1	Target Li-7 fraction, xp	0.999950	0.999950
2	Representative separation factor, alpha	1.045000	1.060000
3	Continuous total stage requirement	167.915832	126.845211
4	Minimum theoretical stages, N	168.000000	127.000000

	Parameter	Electrochemical	COLEX
5	Column 1 stages	10.000000	8.000000
6	Column 2 stages	38.000000	29.000000
7	Column 3 stages	120.000000	90.000000
8	Total cascade stages	168.000000	127.000000
9	Sensitivity alpha — low	1.040000	1.055000
10	Sensitivity stages — low	189.000000	139.000000
11	Sensitivity alpha — representative	1.045000	1.060000
12	Sensitivity stages — representative	168.000000	127.000000
13	Sensitivity alpha — high	1.050000	1.065000
14	Sensitivity stages — high	152.000000	118.000000
15	Operational alpha — low	1.028000	1.043000
16	Predicted enrichment (%) — low	99.921705	99.961395
17	Operational alpha — intermediate	1.036000	1.051000
18	Predicted enrichment (%) — intermediate	99.978700	99.985368
19	Operational alpha — representative	1.045000	1.060000
20	Predicted enrichment (%) — representative	99.995018	99.995045
21	Column 1 actual Li-7 enrichment (%)	95.038031	95.159134
22	Column 2 actual Li-7 enrichment (%)	99.029264	99.069869
23	Column 3 actual Li-7 enrichment (%)	99.995018	99.995045
24	Sequential cascade final enrichment (%)	99.995018	99.995045

```
======================================================================
AUTOMATED CONSISTENCY CHECKS
======================================================================
```

i Baseline stage-value checks skipped because one or more central input parameters were modified.

✓ EC minimum stage requirement = 168

✓ COLEX minimum stage requirement = 127

```
✓ EC cascade distribution = 10 + 38 + 120 = 168
✓ COLEX cascade distribution = 8 + 29 + 90 = 127
✓ Column 1 and Column 2 ceiling operations verified
✓ Column 3 residual-stage allocation verified
✓ EC sequential cascade reaches/exceeds 99.995000% Li-7 target
✓ COLEX sequential cascade reaches/exceeds 99.995000% Li-7

ALL CONSISTENCY CHECKS PASSED.
```

Reproducibility Test 3:

When, $\alpha_{Electrochemical} = 1.050,\ \alpha_{COLEX} = 1.050,\ x_f = 0.9247,\ and\ x_p = 0.99999$;

```
======================================================================
SECTION 4.2 — DETERMINATION OF MINIMUM THEORETICAL STAGE REQUIREMENTS FOR
ELECTROCHEMICAL AND COLEX PROCESSES
======================================================================
```

	Process	Feed fraction xf	Target product fraction xp	Representative alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	0.92470	0.999990	1.050	184.564	185
1	COLEX	0.92470	0.999990	1.050	184.564	185

```
======================================================================
SECTION 5 — CASCADE CONFIGURATION AND STAGE DISTRIBUTION
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Representative separation factor	1.05	1.05
1	Column 1: 92.470000% → 95.000000%	9.00	9.00
2	Column 2: 95.000000% → 99.000000%	34.00	34.00
3	Column 3: 99.000000% → 99.999000%	142.00	142.00
4	Total theoretical stages	185.00	185.00

```
CASCADE CALCULATION DETAILS
----------------------------------------------------------------------
```

	Parameter	Electrochemical	COLEX

	Parameter	Electrochemical	COLEX
0	Overall continuous stage requirement	184.564377	184.564377
1	Overall minimum integer stages N	185.000000	185.000000
2	Column 1 continuous requirement	8.945445	8.945445
3	Column 1 integer stages N1	9.000000	9.000000
4	Column 2 continuous requirement	33.832247	33.832247
5	Column 2 integer stages N2	34.000000	34.000000
6	Column 3 continuous requirement	141.786685	141.786685
7	Column 3 allocated stages N3	142.000000	142.000000
8	Total allocated stages	185.000000	185.000000

==========
SECTION 6 — SENSITIVITY ANALYSIS OF THE IDEAL CASCADES WITH REPRESENTATIVE SEPARATION FACTOR PERTURBATIONS
==========

	Process	Representative alpha	Sensitivity alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	1.050	1.045	204.579	205
1	Electrochemical	1.050	1.050	184.564	185
2	Electrochemical	1.050	1.055	168.188	169
3	COLEX	1.050	1.045	204.579	205
4	COLEX	1.050	1.050	184.564	185
5	COLEX	1.050	1.055	168.188	169

==========
SECTION 7.1 — OPERATIONAL ENRICHMENT PERFORMANCE PREDICTIONS OF THE DESIGNED CASCADES
==========

	Process	Designed stages N	Representative alpha	Evaluated alpha	Predicted final Li-7 enrichment (%)
0	Electrochemical	185	1.050	1.033	99.979948
1	Electrochemical	185	1.050	1.041	99.995187
2	Electrochemical	185	1.050	1.050	99.999021
3	COLEX	185	1.050	1.033	99.979948
4	COLEX	185	1.050	1.041	99.995187
5	COLEX	185	1.050	1.050	99.999021

```
======================================================================
SECTION 7.2 — COLUMN-WISE ACTUAL ENRICHMENT AFTER ROUNDED STAGE ALLOCATION
======================================================================
```

	Parameter	Electrochemical	COLEX
0	Column 1 actual Li-7 enrichment (%)	95.012628	95.012628
1	Column 2 actual Li-7 enrichment (%)	99.010681	99.010681
2	Column 3 actual Li-7 enrichment (%)	99.999021	99.999021

```
======================================================================
SEQUENTIAL CASCADE PERFORMANCE VERIFICATION
======================================================================
```

	Process	Column 1 stages	Column 2 stages	Column 3 stages	Total stages	Final Li-7 enrichment (%)
0	Electrochemical	9	34	142	185	99.999021
1	COLEX	9	34	142	185	99.999021

```
======================================================================
COMPARATIVE INTERPRETATION
======================================================================
✓ EC and COLEX require the same number of theoretical stages.
Stage difference (EC - COLEX) = 0 stages
COLEX requires approximately 0.000% fewer stages than EC.
EC sensitivity range = 36 stages
COLEX sensitivity range = 36 stages
✓ EC and COLEX exhibit the same sensitivity range under the specified
perturbation.
```

```
Enrichment Performance Predictions:
✓ Both processes showed the same enrichment deviation over the evaluated
separation-factor deviation range.
✓ These prediction results indicate the same enrichment performance for the
electrochemical and COLEX processes across all three columns.

================================================================================
INTEGRATED REPRODUCIBLE COMPARATIVE SUMMARY
================================================================================
```

	Parameter	Electrochemical	COLEX
0	Feed Li-7 fraction, xf	0.924700	0.924700
1	Target Li-7 fraction, xp	0.999990	0.999990
2	Representative separation factor, alpha	1.050000	1.050000
3	Continuous total stage requirement	184.564377	184.564377
4	Minimum theoretical stages, N	185.000000	185.000000
5	Column 1 stages	9.000000	9.000000
6	Column 2 stages	34.000000	34.000000
7	Column 3 stages	142.000000	142.000000
8	Total cascade stages	185.000000	185.000000
9	Sensitivity alpha — low	1.045000	1.045000
10	Sensitivity stages — low	205.000000	205.000000
11	Sensitivity alpha — representative	1.050000	1.050000
12	Sensitivity stages — representative	185.000000	185.000000
13	Sensitivity alpha — high	1.055000	1.055000
14	Sensitivity stages — high	169.000000	169.000000
15	Operational alpha — low	1.033000	1.033000
16	Predicted enrichment (%) — low	99.979948	99.979948
17	Operational alpha — intermediate	1.041000	1.041000
18	Predicted enrichment (%) — intermediate	99.995187	99.995187

	Parameter	Electrochemical	COLEX
19	Operational alpha — representative	1.050000	1.050000
20	Predicted enrichment (%) — representative	99.999021	99.999021
21	Column 1 actual Li-7 enrichment (%)	95.012628	95.012628
22	Column 2 actual Li-7 enrichment (%)	99.010681	99.010681
23	Column 3 actual Li-7 enrichment (%)	99.999021	99.999021
24	Sequential cascade final enrichment (%)	99.999021	99.999021

```
================================================================================
AUTOMATED CONSISTENCY CHECKS
================================================================================
i Baseline stage-value checks skipped because one or more central input
parameters were modified.
✓ EC minimum stage requirement = 185
✓ COLEX minimum stage requirement = 185
✓ EC cascade distribution = 9 + 34 + 142 = 185
✓ COLEX cascade distribution = 9 + 34 + 142 = 185
✓ Column 1 and Column 2 ceiling operations verified
✓ Column 3 residual-stage allocation verified
✓ EC sequential cascade reaches/exceeds 99.999000% Li-7 target
✓ COLEX sequential cascade reaches/exceeds 99.999000% Li-7

ALL CONSISTENCY CHECKS PASSED.
```

Reproducibility Test 4:

When, $\alpha_{Electrochemical} = 1.060,\ \alpha_{COLEX} = 1.050,\ x_f = 0.9247,\ and\ x_p = 0.999995$;

```
================================================================================
SECTION 4.2 — DETERMINATION OF MINIMUM THEORETICAL STAGE REQUIREMENTS FOR
ELECTROCHEMICAL AND COLEX PROCESSES
================================================================================
```

	Process	Feed fraction xf	Target product fraction xp	Representative alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	0.92470	0.999995	1.060	166.437	167

	Process	Feed fraction xf	Target product fraction xp	Representative alpha	Continuous stage requirement	Minimum theoretical stages N
1	COLEX	0.92470	0.999995	1.050	198.771	199

==========
SECTION 5 — CASCADE CONFIGURATION AND STAGE DISTRIBUTION
==========

	Parameter	Electrochemical	COLEX
0	Representative separation factor	1.06	1.05
1	Column 1: 92.470000% → 95.000000%	8.00	9.00
2	Column 2: 95.000000% → 99.000000%	29.00	34.00
3	Column 3: 99.000000% → 99.999500%	130.00	156.00
4	Total theoretical stages	167.00	199.00

CASCADE CALCULATION DETAILS

	Parameter	Electrochemical	COLEX
0	Overall continuous stage requirement	166.436591	198.771178
1	Overall minimum integer stages N	167.000000	199.000000
2	Column 1 continuous requirement	7.490268	8.945445
3	Column 1 integer stages N1	8.000000	9.000000
4	Column 2 continuous requirement	28.328673	33.832247
5	Column 2 integer stages N2	29.000000	34.000000
6	Column 3 continuous requirement	130.617649	155.993486
7	Column 3 allocated stages N3	130.000000	156.000000
8	Total allocated stages	167.000000	199.000000

==========
SECTION 6 — SENSITIVITY ANALYSIS OF THE IDEAL CASCADES WITH REPRESENTATIVE SEPARATION FACTOR PERTURBATIONS

	Process	Representative alpha	Sensitivity alpha	Continuous stage requirement	Minimum theoretical stages N
0	Electrochemical	1.060	1.055	181.134	182
1	Electrochemical	1.060	1.060	166.437	167
2	Electrochemical	1.060	1.065	153.999	154
3	COLEX	1.050	1.045	220.326	221
4	COLEX	1.050	1.050	198.771	199
5	COLEX	1.050	1.055	181.134	182

SECTION 7.1 — OPERATIONAL ENRICHMENT PERFORMANCE PREDICTIONS OF THE DESIGNED CASCADES

	Process	Designed stages N	Representative alpha	Evaluated alpha	Predicted final Li-7 enrichment (%)
0	Electrochemical	167	1.060	1.043	99.992801
1	Electrochemical	167	1.060	1.051	99.997990
2	Electrochemical	167	1.060	1.060	99.999516
3	COLEX	199	1.050	1.033	99.987272
4	COLEX	199	1.050	1.041	99.997258
5	COLEX	199	1.050	1.050	99.999506

SECTION 7.2 — COLUMN-WISE ACTUAL ENRICHMENT AFTER ROUNDED STAGE ALLOCATION

Parameter	Electrochemical	COLEX

	Parameter	Electrochemical	COLEX
0	Column 1 actual Li-7 enrichment (%)	95.139211	95.012628
1	Column 2 actual Li-7 enrichment (%)	99.065883	99.010681
2	Column 3 actual Li-7 enrichment (%)	99.999516	99.999506

```
================================================================================
SEQUENTIAL CASCADE PERFORMANCE VERIFICATION
================================================================================
```

	Process	Column 1 stages	Column 2 stages	Column 3 stages	Total stages	Final Li-7 enrichment (%)
0	Electrochemical	8	29	130	167	99.999516
1	COLEX	9	34	156	199	99.999506

```
================================================================================
COMPARATIVE INTERPRETATION
================================================================================
✓ EC requires fewer theoretical stages than COLEX: 167 < 199
Stage difference (EC - COLEX) = -32 stages
COLEX requires approximately -19.162% fewer stages than EC.
EC sensitivity range = 28 stages
COLEX sensitivity range = 39 stages
✓ COLEX is more sensitive to the specified separation-factor variation than
Electrochemical separation.

Enrichment Performance Predictions:
✓ For the same absolute deviation range of the representative separation
factor, COLEX showed a greater ,
enrichment deviation than the electrochemical process.
✓ These prediction results indicate the electrochemical process ,
exhibits higher enrichment in all three columns.

================================================================================
INTEGRATED REPRODUCIBLE COMPARATIVE SUMMARY
================================================================================
```

	Parameter	Electrochemical	COLEX
0	Feed Li-7 fraction, xf	0.924700	0.924700
1	Target Li-7 fraction, xp	0.999995	0.999995
2	Representative separation factor, alpha	1.060000	1.050000
3	Continuous total stage requirement	166.436591	198.771178

	Parameter	Electrochemical	COLEX
4	Minimum theoretical stages, N	167.000000	199.000000
5	Column 1 stages	8.000000	9.000000
6	Column 2 stages	29.000000	34.000000
7	Column 3 stages	130.000000	156.000000
8	Total cascade stages	167.000000	199.000000
9	Sensitivity alpha — low	1.055000	1.045000
10	Sensitivity stages — low	182.000000	221.000000
11	Sensitivity alpha — representative	1.060000	1.050000
12	Sensitivity stages — representative	167.000000	199.000000
13	Sensitivity alpha — high	1.065000	1.055000
14	Sensitivity stages — high	154.000000	182.000000
15	Operational alpha — low	1.043000	1.033000
16	Predicted enrichment (%) — low	99.992801	99.987272
17	Operational alpha — intermediate	1.051000	1.041000
18	Predicted enrichment (%) — intermediate	99.997990	99.997258
19	Operational alpha — representative	1.060000	1.050000
20	Predicted enrichment (%) — representative	99.999516	99.999506
21	Column 1 actual Li-7 enrichment (%)	95.139211	95.012628
22	Column 2 actual Li-7 enrichment (%)	99.065883	99.010681
23	Column 3 actual Li-7 enrichment (%)	99.999516	99.999506
24	Sequential cascade final enrichment (%)	99.999516	99.999506

```
======================================================================
AUTOMATED CONSISTENCY CHECKS
======================================================================
```

i Baseline stage-value checks skipped because one or more central input parameters were modified.

```
✓ EC minimum stage requirement = 167
✓ COLEX minimum stage requirement = 199
✓ EC cascade distribution = 8 + 29 + 130 = 167
✓ COLEX cascade distribution = 9 + 34 + 156 = 199
✓ Column 1 and Column 2 ceiling operations verified
✓ Column 3 residual-stage allocation verified
✓ EC sequential cascade reaches/exceeds 99.999500% Li-7 target
✓ COLEX sequential cascade reaches/exceeds 99.999500% Li-7

ALL CONSISTENCY CHECKS PASSED.
```

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