

Article

First-Principles Modeling of an Electrolytic Cell for Lithium Hydroxide Production: A Multiscale ODE-PDE Framework

Belmiro P. M. Duarte ^{1,2,3,*}  and Nuno M. C. Oliveira ³ 

¹ Polytechnic Institute of Coimbra, Coimbra Institute of Engineering, R. Pedro Nunes, 3030–199 Coimbra, Portugal

² Instituto de Engenharia de Sistemas e Computadores—Coimbra, University of Coimbra, R. Sílvio Lima, Pólo II, 3030–790 Coimbra, Portugal

³ Research Center for Chemical Engineering and Renewable Resources for Sustainability, Department of Chemical Engineering, University of Coimbra, R. Sílvio Lima, Pólo II, 3030–790 Coimbra, Portugal; nuno@eq.uc.pt

* Correspondence: bduarte@isec.pt

Abstract

This study presents a first-principles dynamic model for the electrochemical production of lithium hydroxide (LiOH) in a bench-scale cation exchange membrane (CEM) cell. Its distinguishing feature is a single, dynamically coupled description of the whole cell, in which the lumped Ordinary Differential Equation (ODE) dynamics of the anodic and cathodic chambers are coupled to a spatially resolved Nernst–Planck (PDE) model of membrane ion transport. The model resolves the transient induction period of ion crossover and captures the association kinetics of Li^+ and OH^- , cathodic water reduction, and the back-migration and neutralization of OH^- at the anode, with the local electric field represented by a non-linear potential gradient. Solved by the Method of Lines and reduced through symbolic treatment of the Robin boundary conditions to a consistent ODE system, it yields a numerically robust framework for this stiff, strongly coupled problem. Two process-level results emerge: the membrane strongly attenuates cross-chamber disturbances, largely decoupling the anode and cathode, and it reaches a quasi-steady state far faster than the bulk chambers—a separation of time scales expected to widen at larger volume-to-surface-area ratios. These insights inform scale-up strategies and multiscale control architectures for the cell.

Keywords: process modeling; electrolysis; membrane separation; lithium separation



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1. Introduction

Lithium hydroxide (LiOH) is a critical precursor for high-nickel cathode materials, such as NCM 811 and NCA, which are central to the development of long-range electric vehicles [1–3]. Owing to its relatively low melting point ($\sim 471^\circ\text{C}$), LiOH enables lower-temperature cathode synthesis, thereby preserving the structural integrity and thermal stability of nickel-rich materials [4]. These advantages translate into higher energy densities, extended cycle life, and faster charging performance. As a result, global demand for battery-grade LiOH is increasing rapidly, with major producers projecting annual growth rates of 30–40% [5].

To supply this demand sustainably, membrane electrolytic cells are increasingly adopted to directly convert lithium chloride (LiCl) into battery-grade LiOH. In such systems, LiCl is oxidized at the anode to generate chlorine gas (Cl_2), while water reduction

at the cathode produces hydrogen (H_2) and hydroxide ions (OH^-). Lithium ions migrate selectively through a cation-exchange membrane toward the cathode compartment, where they combine with OH^- to form a high-purity LiOH solution. Compared with conventional processing routes, this electrochemical approach eliminates multi-step causticization, avoids carbonate-based waste generation, and enables the recovery of valuable byproducts such as hydrochloric acid (HCl) [6,7].

Recent research has focused on improving the energy efficiency and product quality of membrane electrolytic systems through cell and membrane optimization. Multiphysics modeling studies demonstrate that adjustments to structural parameters, including electrode spacing and flow-field design, can substantially reduce specific energy consumption [8,9]. Complementary experimental work on advanced membrane materials—such as bilayer and low-fluorine polymeric membranes—has reported high Faradaic efficiencies, reaching up to 94%, alongside enhanced Li^+/Na^+ selectivity [10,11]. Furthermore, parametric analyses of bipolar membrane electrodialysis (BMED) configurations have identified optimal operating regimes in terms of current density and feed composition that consistently meet battery-grade LiOH purity requirements [8,12].

The design and scale-up of these systems increasingly depend on predictive modeling to delineate robust operating windows. Early one-dimensional models provided fundamental insight into concentration polarization and transient ion transport phenomena [13,14]. More recent approaches employ coupled Nernst–Planck and Stefan–Maxwell formulations to resolve localized transport effects, including membrane polarization and hydroxide back-migration [15–18].

Despite these advances, a key limitation persists in the modeling of electrolytic lithium hydroxide production at the system level. Numerous studies have developed detailed cell-scale models that resolve the three-dimensional electrochemical behavior of individual electrolyzers, capturing phenomena such as anode–cathode interactions, ion migration, and membrane transport [12]; however, the constituent domains are typically treated in isolation. What remains lacking is a unified framework that represents the full electrolytic cell as a single, dynamically coupled system—one that simultaneously accounts for the transport and reaction phenomena in the anode and cathode chambers together with the behavior of the ion-selective membrane.

Looking beyond the cell, the eventual goal of facility-scale simulation adds further layers of complexity. A complete industrial description must ultimately integrate downstream and auxiliary units— LiOH crystallization, purification stages, recycle loops for the LiCl and LiOH streams, and the handling or valorization of gaseous byproducts such as Cl_2 and H_2 —within a single framework so that process-wide material and energy recirculation can be assessed, bottlenecks can be identified, and overall plant efficiency and product purity can be optimized. Such plant-wide models, however, can only be as reliable as the cell-level descriptions on which they rest: a dynamically coupled, transport-resolved model of the cell itself is a prerequisite that is currently missing and on which the management of the stringent thermal and chemical balances of industrial-scale, battery-grade LiOH manufacturing ultimately depends [19].

Accordingly, the present work takes the necessary first step toward that broader objective by developing and analyzing a dynamic, first-principles model of a single membrane cell, grounded in a real bench-scale unit. Its aims are threefold: to capture the dominant physico-chemical phenomena governing the unit at this scale; to establish a numerically robust strategy for the resulting stiff, coupled ODE–PDE system; and to extract process-level insight into the cell’s dynamic behavior—notably its characteristic time scales and disturbance sensitivity—that can inform expectations and control requirements as the system is scaled toward prototype and industrial operation. The framework is deliberately confined

to the liquid-phase dynamics of the cell and does not yet incorporate the downstream units or gas-phase recovery outlined above, which are reserved for future extensions.

Novelty Statement and Organization

This work develops a multi-scale, first-principles model for the selective separation of Li^+ from LiCl solutions in a single electrolytic cell equipped with a sulfonic-based cation exchange membrane (CEM). Relative to existing descriptions, it contributes three main elements to electrochemical process modeling:

1. *Hybrid ODE-PDE Coupling:* Coupling the lumped bulk-phase dynamics of the chambers to time-dependent membrane transport equations resolves the transient “induction period” of ion crossover—the finite interval over which the membrane concentration profiles and the crossover flux develop before reaching a steady state. This regime cannot be represented by steady-state models and governs the early-time evolution of the current efficiency.
2. *Parasitic Leakage Dynamics:* Explicit modeling of OH^- back-migration and its neutralization at the anode yields a rigorous, time-resolved estimate of the net current efficiency, beyond what steady-state assumptions allow.
3. *Complexation Kinetics:* Accounting for the finite kinetics of LiOH complex formation provides a more realistic description of the cathode chemistry and of the resulting product composition.

The remainder of this paper is organized as follows: Section 2 provides background information and introduces the dynamic model for Li^+ ion separation. Section 3 details the numerical methods used for the simulations. Section 4 presents the results for a bench-scale electrolysis cell, including an analysis of time constants, disturbance responses, and current efficiency. Finally, Section 5 summarizes the primary findings and highlights this paper’s contributions.

2. Process Modeling

Boldface lowercase letters denote vectors, while boldface uppercase letters represent continuous domains. Blackboard bold uppercase letters are used for discrete domains, and standard uppercase letters denote matrices. Finite sets with ι elements are compactly represented by $[\iota] \equiv \{1, \dots, \iota\}$. The transpose of a vector or matrix is denoted by T .

For notational simplicity, the chemical species OH^- is denoted by OH , Li^+ by Li , the complex $\text{Li}^+ - \text{OH}^-$ by $\text{Li} - \text{OH}$, and lithium hydroxide by LiOH . The electric potential is denoted by Φ , and the electric field is denoted by E_f . Variables used to characterize the cathode, anode, and membrane states are indicated by the superscripts “cat”, “ano”, and “mb”, respectively.

2.1. Process Description

The process aims to model an existing bench-scale unit currently used for experimental trials, with the objective of scaling it up to prototype and industrial applications. The system consists of two chambers—one cathodic and one anodic—separated by a sulfonic (cation-exchange) membrane, forming a conventional electrolytic cell. A schematic representation of the process is shown in Figure 1.

The anode chamber is fed with a fresh LiCl stream at a flow rate of $F_{\text{LiCl}}^{\text{fresh}}$ and a concentration of $C_{\text{LiCl}}^{\text{fresh}}$. Simultaneously, a recycled stream with flow rate $F_{\text{LiCl}}^{\text{rec}}$ and concentration $C_{\text{LiCl}}^{\text{rec}}$ is also supplied. A pure water stream is added to compensate for volumetric losses and for water transport toward the cathode chamber. The operating conditions in the anode chamber ensure that LiCl dissolves rapidly and completely, yielding Li^+ and Cl^- ions. The chloride ions undergo anodic oxidation according to the reaction $2\text{Cl}^- \longrightarrow \text{Cl}_2 + 2\text{e}^-$.

The pH in the anode chamber is typically maintained at a value of approximately 2, which is ensured by acidifying the water feed.

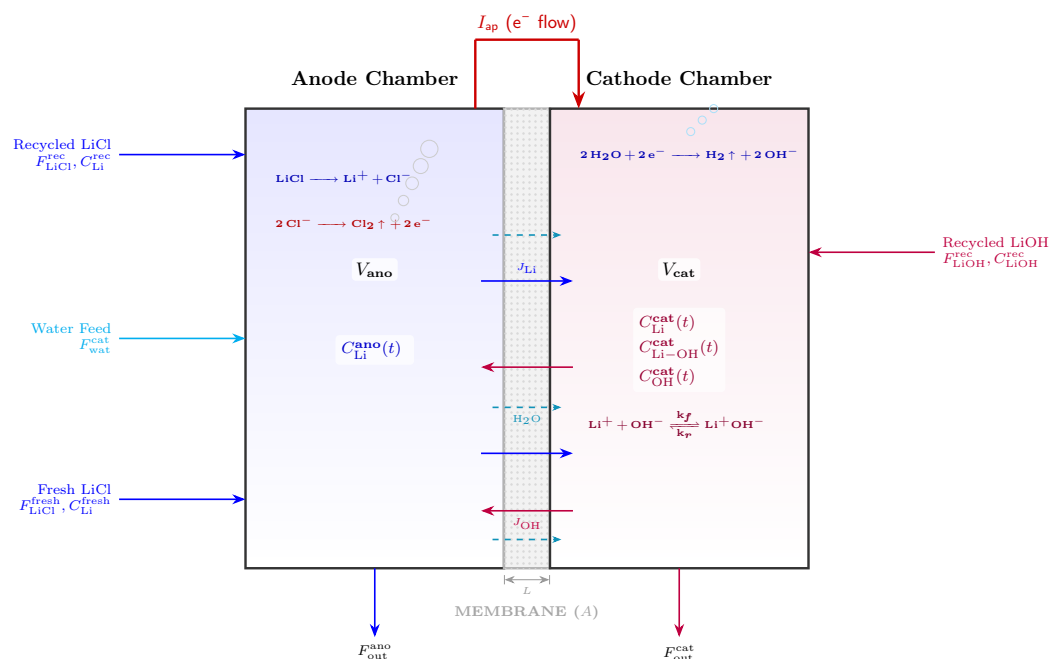


Figure 1. Conceptual representation of the electrolytic cell. The arrows indicate the migration paths of the ionic species: blue arrows denote Li^+ ions, and wine-colored arrows denote OH^- ions.

The concentration of Li^+ in the anode chamber is denoted by $C_{\text{Li}}^{\text{ano}}(t)$, and that of hydroxide is denoted by $C_{\text{OH}}^{\text{ano}}(t)$. A full dynamic balance is retained for $C_{\text{OH}}^{\text{ano}}(t)$ [Equation (2)]; however, the acidification of the water feed buffers the proton concentration at $C_{\text{H}}^{\text{ano}} \approx 10^{-2} \text{ M}$ ($\text{pH} \approx 2$), and the neutralization (water-association) kinetics are very fast ($k_a = 1.4 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$). As a result, the hydroxide balance relaxes almost instantaneously to the quasi-equilibrium condition $C_{\text{H}}^{\text{ano}} C_{\text{OH}}^{\text{ano}} \approx C_{\text{H}_2\text{O}}/K_{\text{wat,eq}}$ so that $C_{\text{OH}}^{\text{ano}}(t)$ is effectively pinned by the autoionization equilibrium at a nearly constant trace value (of order 10^{-12} M), rather than being imposed as constant a priori. The volume of liquid in the anode chamber is denoted by V_{ano} , and the amount of added water is regulated so as to maintain it constant over time.

Perfect mixing conditions are assumed in the anode chamber; therefore, the outlet stream has a flow rate of $F_{\text{out}}^{\text{ano}}$ and concentrations of Li^+ and OH^- equal to $C_{\text{Li}}^{\text{ano}}(t)$ and $C_{\text{OH}}^{\text{ano}}(t)$, respectively. The membrane has thickness L and active area A . Ionic species Li^+ and OH^- are transported across the membrane, with their transport governed by a one-dimensional Nernst–Planck formulation that accounts for both diffusion and electromigration driven by the local electric potential (Figure 2). The spatial and temporal evolution of the ionic concentrations within the membrane are described by $C_{\text{Li}}^{\text{mb}}(x, t)$ and $C_{\text{OH}}^{\text{mb}}(x, t)$, respectively. The electric potential within the membrane is denoted by $\Phi^{\text{mb}}(x, t)$, and the potential difference between the anode and cathode chambers provides the driving force for ionic migration. Electroneutrality is assumed both within the membrane and in the adjacent chambers. The flux of ions at the membrane–chamber interfaces provides boundary conditions for the membrane transport equations and simultaneously acts as a source/sink term for the chamber balances. Membrane selectivity and the possibility of limiting current effects are considered in the model to account for deviations from ideal transport at high applied potentials.

terfacial transport. For a species i in the anode volume V_{ano} , the lumped-parameter mass balance is

$$V_{\text{ano}} \frac{dC_i(t)}{dt} = \sum F_{\text{in}} C_{\text{in}} - \sum F_{\text{out}} C_{\text{out}} + R_i(t) \pm \mathcal{N}_i(t)$$

where $\mathcal{N}_j(t)$ is the total molar transfer rate across the membrane's interface in mol s^{-1} . For the lithium and hydroxide ions, this yields

$$\begin{aligned} \frac{dC_{\text{Li}}^{\text{ano}}(t)}{dt} = & \frac{F_{\text{LiCl}}^{\text{rec}}}{V_{\text{ano}}} (C_{\text{Li}}^{\text{rec}} - C_{\text{Li}}^{\text{ano}}(t)) + \frac{F_{\text{LiCl}}^{\text{fresh}}}{V_{\text{ano}}} (C_{\text{Li}}^{\text{fresh}} - C_{\text{Li}}^{\text{ano}}(t)) - \\ & \frac{F_{\text{wat}}^{\text{ano}}(t)}{V_{\text{ano}}} C_{\text{Li}}^{\text{ano}}(t) - \frac{A J_{\text{Li}}^{\text{ano}}(t)}{V_{\text{ano}}} - \frac{Q_w^{\text{ano}}(t)}{V_{\text{ano}}} C_{\text{Li}}^{\text{ano}}(t), \end{aligned} \quad (1)$$

$$\begin{aligned} \frac{dC_{\text{OH}}^{\text{ano}}(t)}{dt} = & -k_a \left(C_{\text{H}}^{\text{ano}}(t) C_{\text{OH}}^{\text{ano}}(t) - \frac{C_{\text{H}_2\text{O}}}{K_{\text{wat,eq}}} \right) + \frac{A J_{\text{OH}}^{\text{ano}}(t)}{V_{\text{ano}}} - \\ & \frac{F_{\text{wat}}^{\text{ano}}(t)}{V_{\text{ano}}} C_{\text{OH}}^{\text{ano}}(t) - \frac{Q_w^{\text{ano}}(t)}{V_{\text{ano}}} C_{\text{OH}}^{\text{ano}}(t) \end{aligned} \quad (2)$$

where k_a and $K_{\text{wat,eq}}$ represent the water association rate and autoionization equilibrium constants, respectively.

The positive sign for $J_{\text{OH}}^{\text{ano}}$ in Equation (2) accounts for hydroxide crossover from the cathode. The interfacial molar fluxes $J_i^{\text{ano}}(t)$ correspond to the general Nernst–Planck membrane flux (Appendix C, Equation (A14)) evaluated at the anode boundary ($x = 0$).

The volumetric water flow $Q_w^{\text{ano}}(t)$ leaving the anode is driven by the electro-osmotic drag within the hydration shells of migrating lithium ions:

$$Q_w^{\text{ano}}(t) = \frac{n_{\text{hyd}} J_{\text{Li}}^{\text{ano}}(t) A}{C_{\text{H}_2\text{O}}} \quad (3)$$

where n_{hyd} is the lithium hydration number, and $C_{\text{H}_2\text{O}} \approx 55.55 \text{ M}$. The effective diffusivity coefficient for each species i is evaluated as $D_i^{\text{eff}} = D_i \epsilon / \tau$ using the data considered in Table 1.

Table 1. Physical, geometric, and operating parameters for the baseline simulation.

Parameter	Value	Parameter	Value
<i>Physical and thermodynamic parameters</i>			
D_{Li} ($\text{m}^2 \text{s}^{-1}$)	4.11×10^{-10}	D_{OH} ($\text{m}^2 \text{s}^{-1}$)	1.83×10^{-10}
z_{Li}	1	z_{OH}	−1
ϵ (porosity)	0.35	τ (tortuosity)	1.6
k_f ($\text{L mol}^{-1} \text{s}^{-1}$)	1.2×10^6	k_r (s^{-1})	3.2×10^6
k_a ($\text{L mol}^{-1} \text{s}^{-1}$)	1.4×10^8	k_{int} (m s^{-1})	3.0×10^{-4}
n_{hyd}	4.2	$C_{\text{H}_2\text{O}}$ (M)	55.5
R ($\text{J mol}^{-1} \text{K}^{-1}$)	8.314	F (C mol^{-1})	96,485
<i>Geometric and operating parameters</i>			
V_{ano} (L)	15	V_{cat} (L)	7
A (m^2)	1.5×10^{-2}	L (m)	1.5×10^{-4}
$F_{\text{LiCl}}^{\text{rec}}$ (L h^{-1})	192	$F_{\text{LiCl}}^{\text{fresh}}$ (L h^{-1})	0.15
$F_{\text{LiOH}}^{\text{rec}}$ (L h^{-1})	192	T	68 °C (341.15 K)
$C_{\text{LiCl}}^{\text{rec}}$ (M)	3.20	$C_{\text{LiCl}}^{\text{fresh}}$ (M)	11.8
$C_{\text{LiOH}}^{\text{rec}}$ (M)	1.98	I_{ap} (A)	35

2.2.2. Cathode Chamber Balances

In the cathode chamber, lithium, hydroxide, and the aqueous lithium–hydroxide complex ($\text{Li}–\text{OH}$) are governed by the recycle feed, trans-membrane transport, cathodic

water reduction, and complexation kinetics. Assuming perfect mixing in the volume V_{cat} , the mass balances are

$$\frac{dC_{\text{Li}}^{\text{cat}}(t)}{dt} = \frac{F_{\text{Li-OH}}^{\text{rec}}}{V_{\text{cat}}} (C_{\text{Li-OH}}^{\text{rec}} - C_{\text{Li}}^{\text{cat}}(t)) + \frac{AJ_{\text{Li}}^{\text{mb}}(L, t)}{V_{\text{cat}}} - \frac{Q_w^{\text{cat}}(t) - Q_r^{\text{cat}}(t)}{V_{\text{cat}}} C_{\text{Li}}^{\text{cat}}(t) - R_{\text{assoc}}(t), \quad (4a)$$

$$\frac{dC_{\text{OH}}^{\text{cat}}(t)}{dt} = \frac{F_{\text{Li-OH}}^{\text{rec}}}{V_{\text{cat}}} (C_{\text{Li-OH}}^{\text{rec}} - C_{\text{OH}}^{\text{cat}}(t)) + \frac{r_{\text{OH,prod}}(t)}{V_{\text{cat}}} + \frac{AJ_{\text{OH}}^{\text{mb}}(L, t)}{V_{\text{cat}}} - \frac{Q_w^{\text{cat}}(t) - Q_r^{\text{cat}}(t)}{V_{\text{cat}}} C_{\text{OH}}^{\text{cat}}(t) - R_{\text{assoc}}(t), \quad (4b)$$

$$\frac{dC_{\text{Li-OH}}^{\text{cat}}(t)}{dt} = -\frac{F_{\text{Li-OH}}^{\text{rec}}}{V_{\text{cat}}} C_{\text{Li-OH}}^{\text{cat}}(t) - \frac{Q_w^{\text{cat}}(t) - Q_r^{\text{cat}}(t)}{V_{\text{cat}}} C_{\text{Li-OH}}^{\text{cat}}(t) + R_{\text{assoc}}(t) \quad (4c)$$

Interfacial fluxes $J_j^{\text{mb}}(L, t)$ are given by the Nernst–Planck relation (Appendix C, Equation (A14)) evaluated at the cathode interface ($x = L$). Hydroxide is produced locally via the cathodic water reduction ($\text{H}_2\text{O} + \text{e}^- \rightarrow \frac{1}{2} \text{H}_2 + \text{OH}^-$) at a rate of $r_{\text{OH,prod}}(t) = I_{\text{ap}}(t)/F$, where F is the Faraday constant. The net volumetric solvent change in the cathode accounts for the arrival of electro-osmotic water from the anode, $Q_w^{\text{cat}}(t) = Q_w^{\text{ano}}(t)$, and the local consumption of water by a reduction reaction, $Q_r^{\text{cat}}(t)$. The term $-(Q_w - Q_r)/V_{\text{cat}}$ represents the combined effect of dilution (via Q_w) and concentration due to solvent loss (via Q_r). The explicit expression for $Q_r^{\text{cat}}(t)$, the water-consumption coefficient ν_w , and the lithium–hydroxide association rate $R_{\text{assoc}}(t)$ are collected in Appendix C [Equations (A16)–(A17)].

2.2.3. Membrane Balances

We consider the mass balances for Li^+ and OH^- within the membrane domain $x \in [0, L]$, where $x = 0$ denotes the anode interface and $x = L$ denotes the cathode interface. For each species $i \in \{\text{Li}^+, \text{OH}^-\}$, the local conservation of mass is governed by the continuity equation:

$$\frac{\partial C_i^{\text{mb}}(x, t)}{\partial t} = -\frac{\partial J_i^{\text{mb}}(x, t)}{\partial x}$$

By substituting the Nernst–Planck transport equation (Equation (A14)) in this balance, neglecting convection, and considering the effective diffusion coefficients in the membrane's porous structure, we obtain the governing partial differential equations (PDEs) for the following concentrations:

$$\frac{\partial C_{\text{Li}}^{\text{mb}}(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{\text{Li}}^{\text{eff}} \frac{\partial C_{\text{Li}}^{\text{mb}}(x, t)}{\partial x} + \frac{z_{\text{Li}} F}{RT} D_{\text{Li}}^{\text{eff}} C_{\text{Li}}^{\text{mb}}(x, t) \frac{\partial \Phi^{\text{mb}}(x, t)}{\partial x} \right], \quad (5a)$$

$$\frac{\partial C_{\text{OH}}^{\text{mb}}(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{\text{OH}}^{\text{eff}} \frac{\partial C_{\text{OH}}^{\text{mb}}(x, t)}{\partial x} + \frac{z_{\text{OH}} F}{RT} D_{\text{OH}}^{\text{eff}} C_{\text{OH}}^{\text{mb}}(x, t) \frac{\partial \Phi^{\text{mb}}(x, t)}{\partial x} \right] \quad (5b)$$

The species molar fluxes $J_i^{\text{mb}}(x, t)$ appearing in the continuity balance follow from the Nernst–Planck relation. This general flux expression, together with the interfacial (Robin) boundary conditions that couple the membrane to the anode and cathode compartments through the mass-transfer coefficient k_{int} , is collected in Appendix C [Equations (A14) and (A15)].

2.2.4. Potential Distribution and Ohm's Law

The electric potential within the membrane is fundamentally governed by the Poisson equation. However, the extreme sensitivity of Φ to minute local charge imbalances

introduces severe numerical stiffness, requiring prohibitively fine discretization to resolve the space-charge regions [20,21]. To ensure numerical stability while capturing the non-linearities arising from concentration polarization and asymmetric ionic distributions [22,23], we adopt a physics-informed parametrization of the potential profile $\Phi^{\text{mb}}(x, t)$. In the migration-dominant regime, the profile is formally described by a hybrid formulation accounting for interfacial Donnan jumps and the Ohmic drop across the membrane's thickness:

$$\Phi^{\text{mb}}(x, t) = \Phi_{\text{ano}}(t) + \Delta\Phi_D^{\text{ano}}(t) \left(1 - e^{-x/\lambda}\right) + \int_0^x \mathcal{S}(x', t) dx' + \Delta\Phi_D^{\text{cat}}(t) e^{(x-L)/\lambda}$$

where $\Delta\Phi_D^{\text{ano}}(t)$ and $\Delta\Phi_D^{\text{cat}}(t)$ represent the interfacial Donnan potential jumps [24,25], and λ is the characteristic decay length. Here, $\mathcal{S}(x, t)$ represents the bulk gradient of the electric potential. For high-molarity concentrations typical of brine processing (≈ 1.0 M), the bulk membrane resistance dominates the energy landscape, accounting for approximately 90% of the total voltage decrease [26]. Under these conditions, and noting that the potential loss is primarily localized at the anode-side transition and throughout the ionomer bulk, we simplify the derivatives by neglecting the lower-order cathode-side exponential terms. The local electric field and its curvature are thus modeled as:

$$\frac{\partial\Phi^{\text{mb}}(x, t)}{\partial x} \approx \mathcal{S}(x, t) \quad \text{and} \quad \frac{\partial^2\Phi^{\text{mb}}(x, t)}{\partial x^2} \approx \frac{\partial\mathcal{S}(x, t)}{\partial x} \quad (6)$$

To avoid the oversimplification of a constant electric field, the bulk gradient $\mathcal{S}(x, t)$ is not held constant but is derived from the total current density $I(x, t) = F \sum_i z_i I_i(x, t)$ together with the Nernst–Einstein relation ($u_i^{\text{eff}} = D_i^{\text{eff}}/RT$) [27,28]. This keeps the electric field self-consistently coupled to the local concentrations $C_i^{\text{mb}}(x, t)$, capturing the non-uniform conductivity and diffusion potentials critical for high-selectivity lithium extraction [29,30]. The resulting expression for $\mathcal{S}(x, t)$, its spatial derivative $\partial\mathcal{S}/\partial x$ (which reflects the spatial variation in membrane resistance through the local ionic conductivity κ^{mb}), and the associated conductivity terms are reported in Appendix B.

2.3. Integrated System and State Representation

Using a common formalism of process systems engineering [31,32], the individual balances for the chambers and the membrane are grouped into a unified mathematical framework, where the dynamic state of the system is represented by the state vector $\mathbf{x}(t)$:

$$\mathbf{x}(t) = \left(C_{\text{Li}}^{\text{ano}}(t), C_{\text{OH}}^{\text{ano}}(t), C_{\text{Li}}^{\text{cat}}(t), C_{\text{OH}}^{\text{cat}}(t), C_{\text{Li-OH}}^{\text{cat}}(t), C_{\text{Li}}^{\text{mb}}(x, t), C_{\text{OH}}^{\text{mb}}(x, t) \right)^{\text{T}}$$

The variable $C_i^{\text{mb}}(x, t)$ possesses a continuous spatial dependence. However, after the numerical treatment of Section 3, these can be transformed into an approximating finite set of discrete states, corresponding to the specific mesh points of a discretization grid. In addition to the primary state variables, the model characterizes several performance-critical metrics that are algebraically dependent on the state vector $\mathbf{x}(t)$:

- *Electrical Potential:* The spatial distribution $\Phi(x, t)$ is determined by the local ionic conductivity and current density. The field approximation is given by Equation (6), with the full non-linear expressions for the bulk gradient and its curvature reported in Appendix B.
- *Trans-Membrane Water Transport:* The net electro-osmotic water transport leaving the anode is estimated via Equation (3). This term accounts for the electro-osmotic drag effects coupled with the multi-species ionic transport through the membrane.

- **Current Efficiency:** This metric characterizes the effective utilization of the applied current. It is defined by the ratio of the net current contributing to hydroxide production at the cathode to the total applied current, explicitly accounting for Faradaic losses due to OH^- back-migration:

$$\eta(t) = \frac{I_{\text{ap}}(t) - Fz_{\text{OH}}J_{\text{OH}}^{\text{mb}}(L, t)A}{I_{\text{ap}}(t)} \times 100 \quad (7)$$

where $J_{\text{OH}}^{\text{mb}}(L, t)$ represents the interfacial molar flux of species OH and is given by Equation (A14).

The model is further constrained by the principle of local electroneutrality, considering $\sum_i z_i C_i = 0$, to ensure a charge balance across all domains. Furthermore, the coupling between the ionic fluxes $J_i(x, t)$ and the electric field $\partial\Phi/\partial x$ ensures that the total current density remains spatially invariant at any time t , satisfying Kirchhoff's current law across the electrochemical cell.

3. Numerical Treatment

This section details the numerical treatment applied to the coupled transport model described in Section 2. The mathematical framework comprises five ordinary differential equations (ODEs) for lumped chamber dynamics, two one-dimensional partial differential equations (PDEs) for membrane transport, and four algebraic constraints arising from the boundary conditions in Equation (A15).

To mitigate numerical stiffness and enhance the solver stability, the model is converted into non-dimensional form in the spatial and temporal domains, using the transformations

$$x = Lx^* \quad \text{and} \quad t = L^2/D_{\text{Li}}^{\text{eff}}t^*$$

where $x^* \in [0, 1]$ and $t^* \geq 0$ denote the dimensionless independent variables. In this analysis, state variables were maintained in dimensional form to preserve physical transparency, since they already have low magnitude values. The complete dimensionless system is provided in Appendix A.

The computational implementation utilizes the Julia v.1.12.5 programming language, and the ModelingToolkit.jl (MTK) v.1.45.1 high-performance symbolic-numeric modeling framework [33]. Spatially dependent membrane concentrations, $C_i^{\text{mb}}(x^*, t^*)$, are discretized via the Method of Lines (MOL) using MethodOfLines.jl v.0.10.4 [34]. Specifically, an upwind scheme combined with fourth-order finite difference approximations is employed for spatial discretization to suppress numerical dispersion while maintaining high-order accuracy. The domain is partitioned into $N - 1$ equal intervals, yielding N discrete points, which transforms the original PDE-DAE system into a high-dimensional system of differential algebraic equations (DAEs).

To improve computational efficiency, the MTK's `structural_simplify` routine is applied to perform symbolic index reduction and alias elimination. During this process, MTK automatically generates an analytical sparse Jacobian, which significantly accelerates the convergence of Newton iterations within the stiff solver. Algebraic variables associated with the boundary conditions are symbolically solved and substituted into the dynamic equations, reducing the DAE system to a consistent set of ODEs. Finally, the system is integrated using the CVODE_BDFsolver from the Sundials.jl v6.2.2 package [35]. This integrator employs an implicit, variable-order, variable-step backward differentiation formula (BDF) method with a user-defined relative tolerance of 10^{-6} , specifically chosen for the stiff numerical characteristics of electrochemical transport models.

The numerical simulation follows a multi-stage execution pipeline. First, a consistent initial condition is established to satisfy the underlying algebraic constraints of the DAE system. The system is then integrated until it converges to a stationary point, representing the process's steady state. This initialization phase is performed using the `steady_state` solver [36], ensuring that the temporal derivatives $\dot{\mathbf{x}}(t)$ effectively vanish before further analysis.

Once a robust steady-state baseline is established, dynamic simulations are conducted to evaluate the system's resilience and sensitivity. This phase involves introducing step changes and periodic disturbances in the critical input variables—such as the applied current density I_{ap} and feed concentrations—to quantify their transient impact on the state vector $\mathbf{x}(t)$ and associated performance metrics. The post-processing stage involves extracting the time-series solutions and performing a re-dimensionalization to map the dimensionless variables back to their physical units. This step facilitates the calculation of derived figures of merit, specifically the instantaneous current efficiency and the net trans-membrane water transport. Finally, these results are visualized to establish correlations between the distributed spatial dynamics within the membrane and the lumped transient behavior of the anode and cathode chambers.

4. Numerical Results and System Analysis

This section presents the simulation results derived from the mathematical model detailed in Section 2, implemented using the numerical methodology described in Section 3. The presentation begins with an overview of the physical and operational parameters utilized to establish the baseline simulation. Subsequently, the system is analyzed in Section 4.2 to identify the dominant physical phenomena and determine the characteristic time constants. Building upon this foundation, Section 4.3 presents and discusses the dynamic response of the system to typical process disturbances.

4.1. Physical Parameters and Baseline Conditions

The model characterizes a bench-scale electrolytic cell under controlled laboratory settings. The physical, geometric, and operating parameters defining the system are detailed in Table 1. These values represent the reference state for the numerical study, and any deviations during sensitivity analyses are explicitly noted in the relevant sections. These parameters are drawn from the literature and from independent physicochemical sources; no calibration against unit-specific measurements was performed. The results reported below should therefore be read as physically grounded, structural predictions of the cell's dynamic behavior rather than as experimentally validated quantitative forecasts. A quantitative comparison against continuous bench-scale records, using an efficiency definition matched to Equation (7), is identified as the immediate next step (Section 5).

To define the *baseline simulation conditions*, several foundational assumptions are adopted. First, a reference operating point is obtained by solving the model at steady state—that is, by setting all temporal derivatives to zero—using the steady-state solver described in Section 3. This stationary solution is not itself the object of study; it provides a consistent initial condition from which the dynamic simulations are launched, with the transient response to input disturbances analyzed in Section 4.3. The baseline is anchored on the recirculation-stream concentrations C_{LiCl}^{rec} and C_{LiOH}^{rec} (Table 1), which serve as the primary benchmarks for evaluating lithium recovery efficiency. Second, *isothermal operation* at 341.15 K is assumed; this presumes an effective thermal-management system capable of dissipating the Joule heating and reaction enthalpies, which is plausible here given the significant liquid volumes of both the anode and cathode chambers (Table 1). Finally, *invariant electrolyte volumes* are maintained in both chambers: the water feed rate

to the anode, $F_{\text{wat}}^{\text{ano}}(t)$, is dynamically adjusted to compensate for water consumption and osmotic transport across the membrane, with analogous make-up in the cathode.

4.2. System Analysis and Dominant Dynamics

To identify the dominant dynamics governing the electrolytic cell, we evaluate the characteristic time constants (τ) associated with the primary transport and relaxation phenomena. The fundamental transport capability of the membrane is characterized by an effective ionic conductivity ($\sigma_{\text{mb}} \approx 5 \text{ S m}^{-1}$), established via the Nernst–Einstein framework using baseline species concentrations and their effective diffusion coefficients within the hydrated polymer matrix. This value, combined with the vacuum permittivity ($\epsilon_0 \approx 8.854 \times 10^{-12} \text{ F m}^{-1}$) and the effective permittivity of confined water ($\epsilon_{\text{mb}} \approx 25$), defines the most rapid relaxation processes in the system.

Table 2 summarizes these time constants, calculated using the baseline parameters and system geometry defined in Section 4.1. For the electromigrative response, a nominal potential drop of $\Delta\Phi = 0.035 \text{ V}$ is assumed. In industrial-scale applications, this driving force is typically two orders of magnitude higher; since τ_{mig} scales with $L^2/\Delta\Phi$, the acceleration of the migration response remains pronounced even if the membrane thickness L is moderately increased. Consequently, field-driven transport remains the fastest mass-transfer mechanism within the membrane domain.

Table 2. Characteristic time constants for the primary physical phenomena (baseline).

Phenomenon	Expression	Value [s]	Physical Interpretation
Chamber residence (anode)	$\tau_{\text{ano}} = \frac{V_{\text{ano}}}{F_{\text{LiCl}}^{\text{rec}}}$	2.81×10^2	Global renewal rate of the LiCl feed electrolyte
Chamber residence (cathode)	$\tau_{\text{cat}} = \frac{V_{\text{cat}}}{F_{\text{LiOH}}^{\text{rec}}}$	1.31×10^2	Global renewal rate of the LiOH product stream.
Membrane diffusion (Li^+)	$\tau_{\text{diff,Li}} = \frac{L^2}{D_{\text{Li}}^{\text{eff}}}$	2.50×10^2	Diffusive relaxation time for lithium ions in the membrane
Membrane diffusion (OH^-)	$\tau_{\text{diff,OH}} = \frac{L^2}{D_{\text{OH}}^{\text{eff}}}$	5.62×10^2	Diffusive relaxation time for hydroxide ions in the membrane
Membrane migration (Li^+)	$\tau_{\text{mig,Li}} = \frac{L^2 RT}{FD_{\text{Li}}^{\text{eff}} \Delta\Phi}$	2.09×10^2	Electromigrative response of Li^+ to the electric field
Membrane migration (OH^-)	$\tau_{\text{mig,OH}} = \frac{L^2 RT}{FD_{\text{OH}}^{\text{eff}} \Delta\Phi}$	4.72×10^2	Electromigrative response of OH^- to the electric field
Charge relaxation	$\tau_{\text{ohm}} = \frac{\epsilon_0 \epsilon_{\text{mb}}}{\sigma_{\text{mb}}}$	4.43×10^{-11}	Instantaneous adjustment of the electric potential in the membrane
Li–OH formation	$\tau_{\text{Li–OH}} = \frac{1}{k_r}$	3.13×10^{-7}	Formation of Li–OH in the cathode

A comparison of the calculated magnitudes reveals a distinct hierarchy of temporal scales. The charge relaxation time (τ_{ohm}) represents the Maxwell–Wagner relaxation time; its extremely low value ($4.43 \times 10^{-11} \text{ s}$) proves that any local charge imbalance is neutralized almost instantly compared to the millisecond-to-second scales of diffusion and migration. This provides a rigorous physical justification for the electroneutrality approximation ($c_+ = c_-$) in the membrane bulk and a quasi-steady-state assumption regarding the electric potential distribution. Simultaneously, the time scale for the formation of Li–OH in the cathode ($\tau_{\text{Li–OH}}$) is very small, leading to very fast chemical equilibrium for these reactions.

Due to the chamber hydraulic residence times ($\tau_{\text{ano}}, \tau_{\text{cat}}$) chosen, which significantly exceed the remaining time constants, the system exhibits clear temporal decoupling. The global transient response is dictated by the macroscopic volume turnover, while the membrane dynamics remain locally stationary and respond relatively fast to variations in the bulk electrolyte. This is a consequence of the significant liquid volumes present in both chambers, which can be modified as design parameters, for instance, in larger-scale operations.

4.3. Dynamic Simulation Results

This section presents the results of the dynamic simulations obtained with the mathematical model described in Section 2. The simulation protocol began with a physics-informed initialization that was integrated until a stable steady state was established. The system was then subjected to a sequence of step disturbances in various input variables to evaluate its dynamic response. To ensure a complete transition between regimes, disturbances were separated by a relaxation period of 30θ , where $\theta = L^2/D_{\text{Li}}^{\text{eff}} = 4.167$ min represents the characteristic diffusion time across the membrane. Note that the initial interval $[0, 10\theta]$ of the simulation is omitted from the figures to focus exclusively on the transient behavior following the first steady state.

The resulting system behavior is visualized in a 3×2 grid of plots. The upper left panel displays the concentration dynamics of $C_{\text{Li}}^{\text{cat}}(t)$, $C_{\text{Li}}^{\text{ano}}(t)$, $C_{\text{Li-OH}}^{\text{cat}}(t)$, and $C_{\text{OH}}^{\text{cat}}(t)$. The concentration $C_{\text{OH}}^{\text{ano}}(t)$ is not visible in these plots, since it remains negligible (on the order of 10^{-12} M) due to the rapid neutralization reaction at the anode. This right panel also includes the spatial concentration profiles within the membrane, $C_{\text{Li}}^{\text{mb}}(x)$ and $C_{\text{OH}}^{\text{mb}}(x)$, captured at the final steady state.

The middle panel employs 3D surface plots to illustrate the spatiotemporal evolution of $C_{\text{Li}}^{\text{mb}}(x, t)$ and $C_{\text{OH}}^{\text{mb}}(x, t)$, highlighting how internal gradients adjust to external perturbations across the (x, t) domain. The lower panel tracks the dynamics of the electro-osmotic water transport rate leaving the anode—calculated via Equation (3)—and the instantaneous current efficiency determined by Equation (7). All simulations were performed with $N = 51$ discretization points, equivalent to a spatial resolution of $3 \mu\text{m}$ in the membrane.

The first numerical experiment examined the system's response to step disturbances in three primary operational inputs: (i) the LiCl concentration in the anode recycle stream ($C_{\text{LiCl}}^{\text{rec}}$); (ii) the LiOH concentration in the cathode recycle stream ($C_{\text{LiOH}}^{\text{rec}}$); and (iii) the flowrate of LiCl in the anode ($F_{\text{LiCl}}^{\text{rec}}$). The simulation spanned a total duration of 120θ (8.33 h), following these chronological regimes:

1. *Baseline Steady State* : For $t \in [0, 30\theta]$ (2.08 h), the system was maintained at stationary conditions: $C_{\text{LiCl}}^{\text{rec}} = 3.2$ M, $C_{\text{LiOH}}^{\text{rec}} = 1.98$ M, and $I_{\text{ap}} = 35$ A.
2. *Disturbance Phase I*: At $t = 30\theta$, a step increase to $C_{\text{LiCl}}^{\text{rec}} = 3.52$ M was introduced. This phase spanned $t \in [30\theta, 60\theta]$.
3. *Disturbance Phase II*: At $t = 60\theta$, $C_{\text{LiCl}}^{\text{rec}}$ was restored to the baseline, and a step increase to $C_{\text{LiOH}}^{\text{rec}} = 2.178$ M was implemented for $t \in [60\theta, 90\theta]$.
4. *Disturbance Phase III*: At $t = 90\theta$, $C_{\text{LiOH}}^{\text{rec}}$ was restored to the baseline and a step decrease to $F_{\text{LiCl}}^{\text{rec}} = 0.0453 \text{ L s}^{-1}$ was introduced (corresponding to -15%), lasting until $t = 120\theta$.

The results for this experiment are presented in Figure 3, where vertical dashed lines indicate the onset of each disturbance. In panel (a), the four legend entries render as three distinguishable curves, because the cathodic $C_{\text{Li}}^{\text{cat}}$ and $C_{\text{OH}}^{\text{cat}}$ traces nearly coincide and overlap into a single visible line. Two features of the cathode chemistry account for this. First, Li^+ and OH^- enter the chamber in an approximately 1:1 ratio—the recycled LiOH stream supplies both in equal proportion, while the membrane Li^+ influx and the faradaic OH^- production are comparatively small—and the association reaction $\text{Li}^+ + \text{OH}^- \rightleftharpoons \text{Li-OH}$ removes them in strict 1:1 stoichiometry, so it enters the $C_{\text{Li}}^{\text{cat}}$ and $C_{\text{OH}}^{\text{cat}}$ balances identically and cannot by itself create a net imbalance between them. Second, this reaction is essentially instantaneous ($\tau_{\text{Li-OH}} = 1/k_r \approx 3 \times 10^{-7}$ s, Table 2), so it remains close to equilibrium, $C_{\text{Li-OH}}^{\text{cat}} \approx K_{\text{eq}} C_{\text{Li}}^{\text{cat}} C_{\text{OH}}^{\text{cat}}$ with $K_{\text{eq}} = k_f/k_r$, which slaves the neutral complex to the product of the two ionic concentrations and places $C_{\text{Li-OH}}^{\text{cat}}$ on its own, lower curve. The residual difference $C_{\text{Li}}^{\text{cat}} - C_{\text{OH}}^{\text{cat}}$ is therefore set only by the small mismatch between the Li^+ and OH^- interfacial fluxes and the faradaic OH^- source, damped by the strong recycle flushing; the

two remain close rather than exactly equal, as they are integrated as independent states. *Disturbance Phase I* shows that increasing the anode LiCl feed significantly impacts $C_{\text{Li}}^{\text{ano}}$, while the effect on the cathodic species ($C_{\text{Li}}^{\text{cat}}$, $C_{\text{OH}}^{\text{cat}}$, and $C_{\text{Li-OH}}^{\text{cat}}$) remains negligible. This weak inter-chamber coupling is confirmed in *Disturbance Phase II*, where perturbations in the cathodic OH^- concentration do not propagate to the anode, as elucidated by the spatiotemporal profiles in Figure 3c,d. The membrane effectively attenuates disturbance propagation: the Li^+ gradient is dissipated within the membrane thickness, while migrating OH^- ions are immediately neutralized by H^+ at the anode interface, effectively isolating the compartments. In *Disturbance Phase III*, the 15 % decrease in $F_{\text{LiCl}}^{\text{rec}}$ yields no visible change in bulk concentrations, indicating a high system buffer capacity.

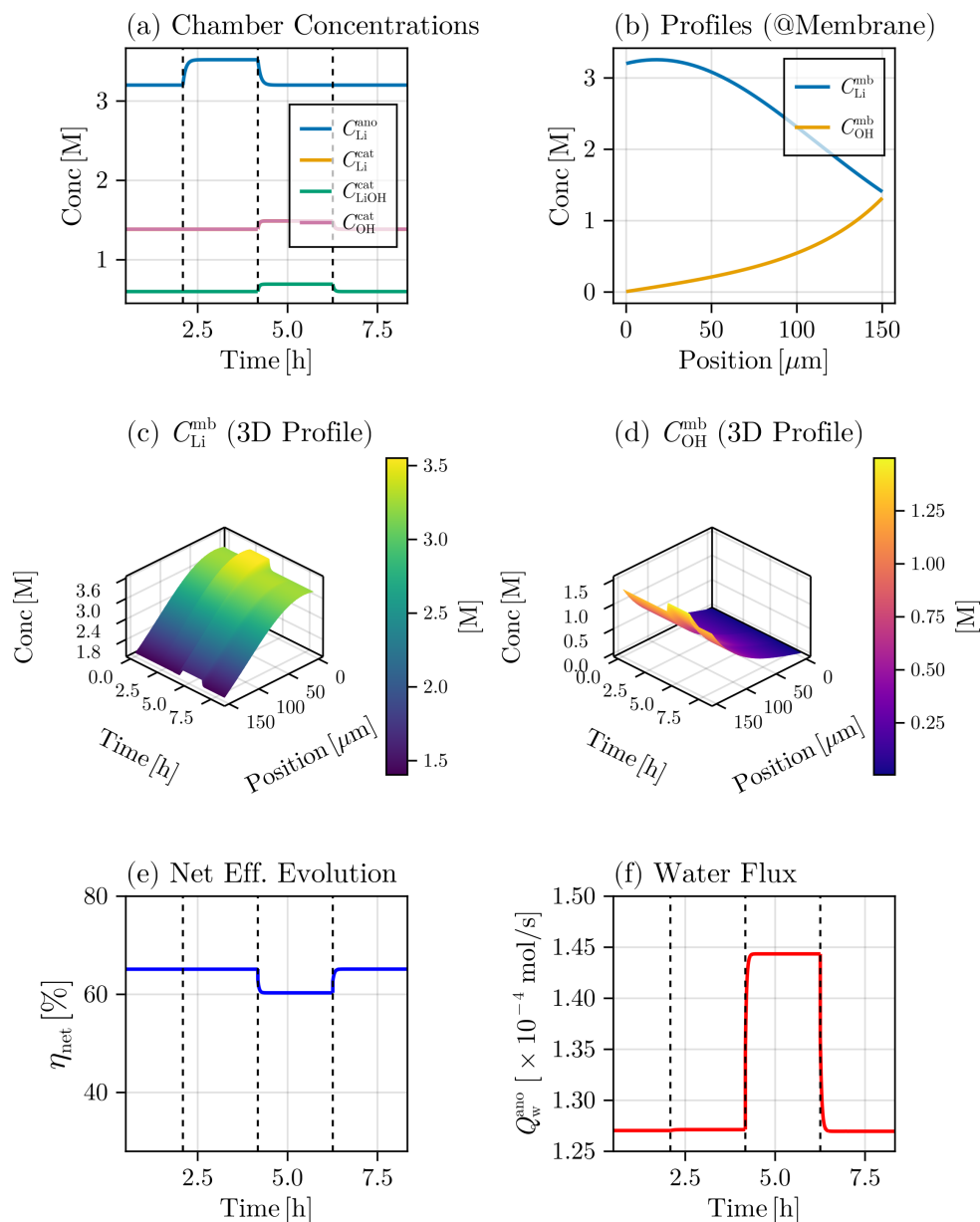


Figure 3. System dynamic response to step disturbances in the concentrations and flowrates: (a) temporal evolution of chamber concentrations; (b) spatial profiles of membrane ion concentrations at the final steady state; (c) spatiotemporal evolution of $C_{\text{Li}}^{\text{mb}}(x, t)$; (d) spatiotemporal evolution of $C_{\text{OH}}^{\text{mb}}(x, t)$; (e) instantaneous current efficiency; and (f) electro-osmotic water transport rate $Q_w^{\text{ano}}(t)$ leaving the anode. In panel (a), the $C_{\text{Li}}^{\text{cat}}$ and $C_{\text{OH}}^{\text{cat}}$ curves nearly coincide and therefore appear as a single trace.

Regarding process efficiency, panel (e) shows that an elevated $C_{\text{OH}}^{\text{cat}}$ reduces η_{net} by enhancing OH^- back-migration. The electro-osmotic water transport in panel (f) exhibits a near-symmetrical relationship with the current efficiency: through (3), the water leaving the anode is set by the lithium flux $J_{\text{Li}}^{\text{ano}}$, and a higher $J_{\text{Li}}^{\text{ano}}$ accompanies a larger LiOH production in the cathode, albeit at a lower current efficiency. Whereas anodic fluctuations (*Disturbance Phase I*) have a negligible impact on water transport, the cathodic perturbations of *Disturbance Phase II* induce a marked increase in it. Finally, the system's dynamic response confirms its inherent stability, as all state variables converge to new steady-state values after an initial transient phase.

The second numerical experiment investigated the system's response to sequential step disturbances in the applied current (I_{ap}). The simulation spanned a total duration of 1500 (10.42 h), following these chronological regimes:

1. *Baseline Steady State*: For $t \in [0, 300]$ (2.08 h), the system was maintained at stationary conditions with $I_{\text{ap}} = 35$ A.
2. *Disturbance Phase I*: For $t \in [300, 600]$, a step increase to $I_{\text{ap}} = 43.75$ A (a +25 % disturbance) was introduced.
3. *Disturbance Phase II*: For $t \in [600, 900]$, the applied current was further increased to $I_{\text{ap}} = 52.5$ A (a +50 % disturbance).
4. *Disturbance Phase III*: For $t \in [900, 1200]$, I_{ap} was decreased to 26.25 A, corresponding to a −25 % disturbance relative to the baseline.
5. *Disturbance Phase IV*: For $t \in [1200, 1500]$, the current was further reduced to $I_{\text{ap}} = 17.5$ A, representing a −50 % disturbance.

The results obtained in this case are presented in Figure 4. As in Figure 3, the $C_{\text{Li}}^{\text{cat}}$ and $C_{\text{OH}}^{\text{cat}}$ curves nearly coincide—owing to the 1:1 supply and consumption of Li^+ and OH^- in the cathode—and appear as a single trace. Compared with the baseline solution, Figure 4a,b shows that both the temporal and the spatial profiles remain almost constant during these perturbations. In particular, $C_{\text{OH}}^{\text{cat}}(t)$ stays largely unchanged, since it is dominated by the value already present in the recycled stream, despite the variations in the rate of OH^- production in the cathode. Consequently, the plots in Figure 5 become useful for analyzing the impact of these disturbances on the current efficiency and the cell productivity.

An increase in I_{ap} effectively increases $C_{\text{OH}}^{\text{cat}}$, although this change is attenuated by the already large value in the cathode. The associated increase in the molar loss across the membrane is therefore very small, as shown in Figure 5a. This leaves the negative term in the numerator of Equation (7) almost unchanged, so the current efficiency increases with I_{ap} , as observed in Figure 4e. Figure 5b shows the variations in the LiOH production rate following these I_{ap} steps. Since $C_{\text{LiOH}}^{\text{rec}}$ is also significant, the instantaneous molar net output flow of LiOH in the cathode chamber shown in this figure is computed as

$$\dot{N}_{\text{LiOH}}^{\text{prod}}(t) = F_{\text{cat}}^{\text{out}}(t) C_{\text{LiOH}}^{\text{cat}}(t) - F_{\text{LiOH}}^{\text{rec}}(t) C_{\text{LiOH}}^{\text{rec}}(t).$$

The changes introduced in I_{ap} induce variations of approximately 15 % to 20 % in $\dot{N}_{\text{LiOH}}^{\text{prod}}$, with corresponding variations in the current efficiency. Hence, the predictive capability of this model makes it advantageous for optimizing the design and the choice of operating conditions of these cells.

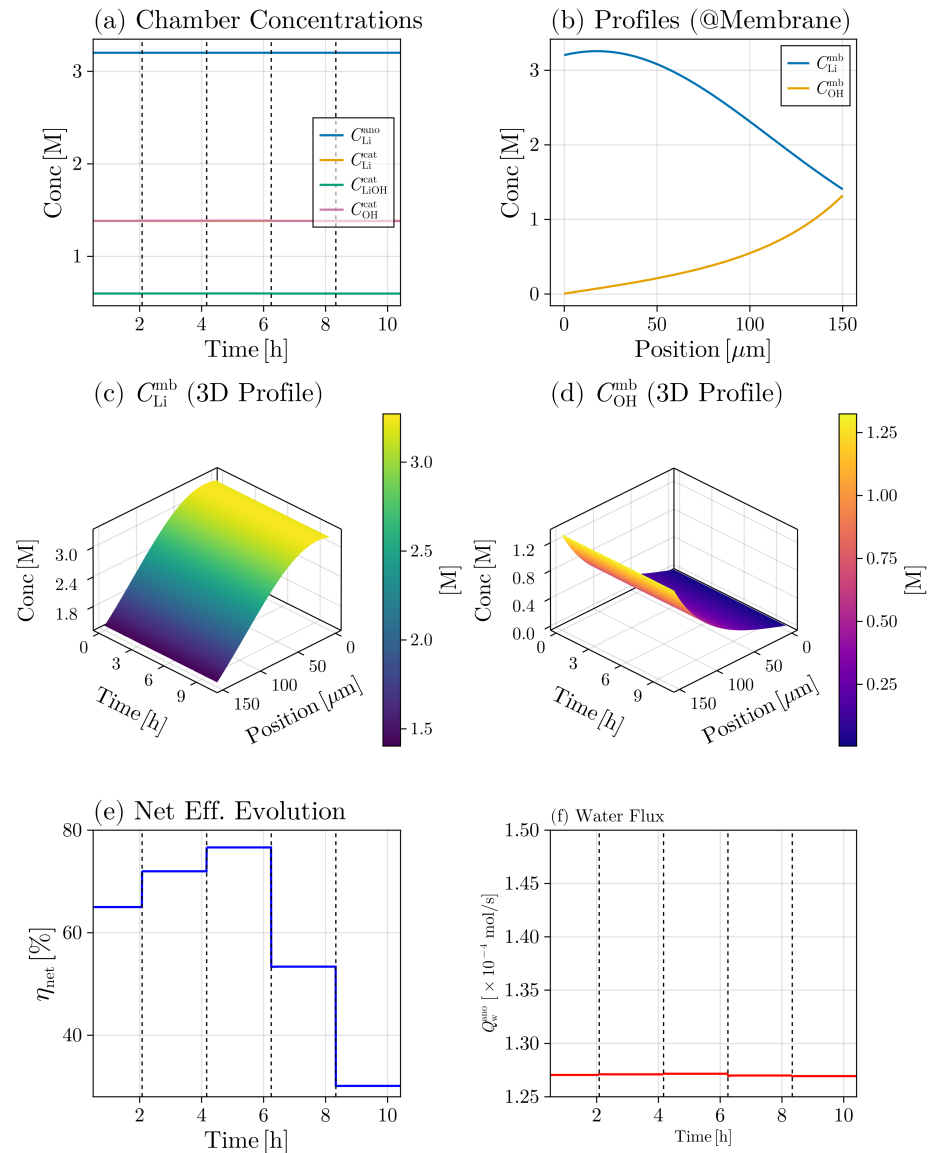


Figure 4. System dynamic response to step disturbances in the current intensity: (a) temporal evolution of chamber concentrations; (b) spatial profiles of membrane ion concentrations at the final steady state; (c) spatiotemporal evolution of $C_{Li}^{mb}(x, t)$; (d) spatiotemporal evolution of $C_{OH}^{mb}(x, t)$; (e) instantaneous current efficiency; and (f) electro-osmotic water transport rate $Q_w^{ano}(t)$ leaving the anode. In panel (a), the C_{Li}^{cat} and C_{OH}^{cat} curves nearly coincide and therefore appear as a single trace.

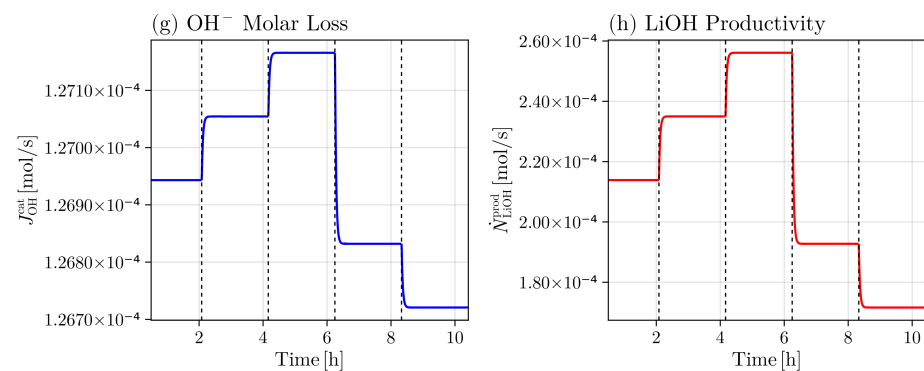


Figure 5. Dynamic evolution of (a) the loss of OH^- across the membrane and (b) the net output flow of LiOH in the cathode chamber.

To further evaluate the system's sensitivity, a third numerical experiment investigated the influence of the values of the flow, transport, and environmental parameters: (i) the LiCl recycle flow ($F_{\text{LiCl}}^{\text{rec}}$); (ii) the operating temperature (T); and (iii) the external mass transfer coefficient (k_{int}). Adhering to the established chronological protocol (120 θ), we have the following:

1. *Baseline Steady State*: For $t \in [0, 30\theta]$, the system was held at $F_{\text{LiCl}}^{\text{rec}} = 192 \text{ L h}^{-1}$, $T = 341.15 \text{ K}$, and $k_{\text{int}} = 3 \times 10^{-4} \text{ m s}^{-1}$.
2. *Disturbance Phase I*: At $t = 30\theta$, $F_{\text{LiCl}}^{\text{rec}}$ was increased by 10 % to 211.2 L h^{-1} .
3. *Disturbance Phase II*: At $t = 60\theta$, the flow was restored, and the temperature was increased to $T = 351.15 \text{ K}$.
4. *Disturbance Phase III*: At $t = 90\theta$, the temperature was restored and the mass transfer coefficient was increased to $k_{\text{int}} = 6 \times 10^{-4} \text{ m s}^{-1}$.

The results, presented in Figure 6, illustrate a possible coupling between the transport parameters and the electrochemical performance of the cell. As in Figures 3 and 4, the $C_{\text{Li}}^{\text{cat}}$ and $C_{\text{OH}}^{\text{cat}}$ curves nearly coincide and appear as a single trace. The bulk chamber concentrations remain remarkably stable despite disturbances in $F_{\text{LiCl}}^{\text{rec}}$, T , and k_{int} . The insensitivity to $F_{\text{LiCl}}^{\text{rec}}$ stems from the high recycle ratio, which keeps the chambers well-mixed and dominated by the reaction–migration balance. Because the reaction kinetics are modeled as temperature-independent, thermal effects are manifested primarily through membrane transport, particularly electromigration; consequently, the temperature step induces no discernible change in the bulk states or the membrane concentration profiles [plots (c) and (d)]. We note that the model does not yet include an explicit temperature dependence of the diffusion coefficients, which would likely intensify this trend in a real-world scenario.

The external mass-transfer coefficient (k_{int}) has only a small, second-order effect on electro-osmotic water transport, which, in the model, is the water carried out of the anode chamber by the hydration shells of the migrating Li^+ ions [Equation (3)], evaluated from the anode-side flux $J_{\text{Li}}^{\text{mb}}(0, t)$. A larger k_{int} lowers the interfacial resistance and suppresses OH^- back-migration, improving the net current efficiency. Its effect on water transport is more subtle: raising k_{int} pins the membrane interfacial concentration $C_{\text{Li}}^{\text{mb}}(0, t)$ closer to the anode bulk value $C_{\text{Li}}^{\text{ano}}(t)$, narrowing the driving concentration difference in the Robin condition [Equation (A15a)]. Under the fixed applied current, the net anode-side lithium flux is thereby slightly reduced, and, through the hydration coupling [Equation (3)], the electro-osmotic water leaving the anode—and hence reaching the cathode—decreases marginally.

It is worth clarifying the origin of this reduction at the continuum level resolved by the model. Because the interfacial concentration $C_{\text{Li}}^{\text{mb}}(0, t)$ and the local field gradient $\mathcal{S}(x, t)$ are both resolved [Equation (6) and Appendix B], the two candidate causes can be distinguished directly. The increase in k_{int} produces only a modest shift in the interfacial lithium concentration, of order 1 % at $x = 0$, and a correspondingly small adjustment of the field within the membrane bulk, with no sharp concentration-polarization layer. The reduced water transport is therefore a driving-force effect—the slightly lower interfacial lithium flux and the associated field adjustment—rather than a change in the membrane hydration state. This attribution is, however, a property of the present formulation, which carries a constant hydration number [Equation (3)] and no water-activity variable: microscopic effects such as localized interfacial dehydration or a drop in water activity lie outside its resolution and would require a composition- and potential-dependent hydration number or an explicit Maxwell–Stefan treatment of water as a transported species. A further channel neglected here is the water carried with OH^- during back-migration; like the refinements above, it is a second-order effect not expected to change the small magnitude observed.

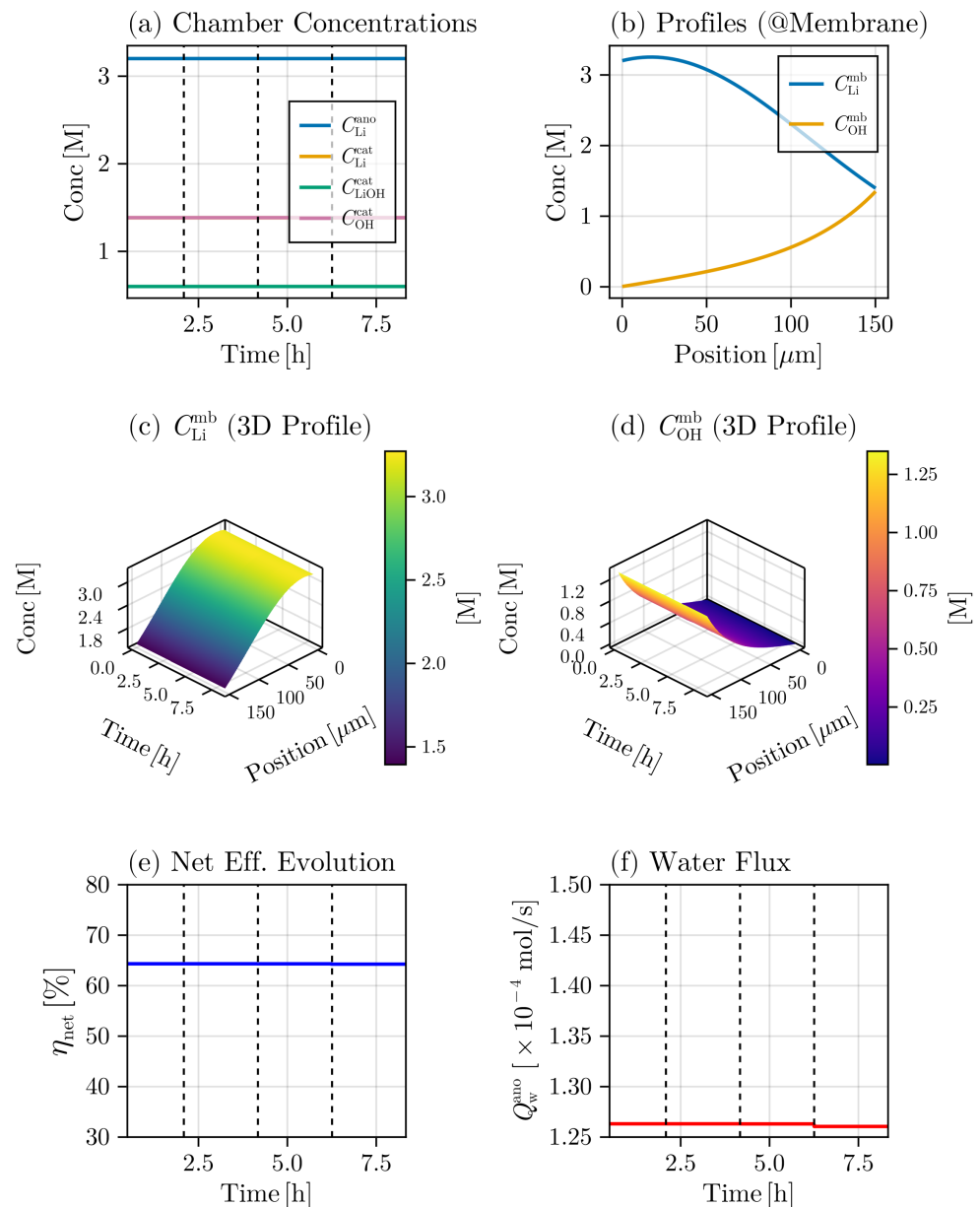


Figure 6. Dynamic sensitivity analysis for the transport and environmental parameters: (a) temporal concentration profiles in the anode and cathode chambers; (b) steady-state spatial profiles of membrane species; (c) spatiotemporal evolution of $C_{Li}^{mb}(x, t)$; (d) spatiotemporal evolution of $C_{OH}^{mb}(x, t)$; (e) net current efficiency (η_{net}) response; and (f) electro-osmotic water transport rate $Q_w^{ano}(t)$ leaving the anode. In panel (a), the C_{Li}^{cat} and C_{OH}^{cat} curves nearly coincide and therefore appear as a single trace.

5. Conclusions

This work supports four main conclusions.

First, a single, dynamically coupled ODE-PDE model of the complete CEM cell was formulated and solved. A symbolic reduction in the Robin boundary conditions yielded a consistent, numerically robust ODE system for this stiff, strongly coupled problem.

Second, the cell behaves as a largely decoupled system, with the membrane acting as a high-order, low-pass filter between the chambers. The anode and cathode can therefore be optimized and controlled independently.

Third, membrane transport and interfacial mass transfer are the dominant levers on net current efficiency. They set the rates of OH^- back-migration and of electro-osmotic water transport toward the cathode.

Fourth, the membrane reaches a quasi-steady state much faster than the bulk chambers. This separation of time scales should widen at larger volume-to-surface-area ratios, motivating a multiscale control strategy for scaled-up units.

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Data Availability Statement: The data supporting the findings of this study are available within this article. The source code used to generate the numerical results is available from the corresponding author upon reasonable request.

Conflicts of Interest: The authors declare no conflicts of interest.

Nomenclature

Latin symbols

A	Membrane active area (m^2)
C_i^j	Concentration of species i in domain $j \in \{\text{ano, cat, mb}\}$ (M)
$C_{\text{H}_2\text{O}}$	Molar concentration of water (M)
D_i, D_i^{eff}	Free-solution and effective diffusion coefficient of species i ($\text{m}^2 \text{s}^{-1}$)
F	Faraday constant (C mol^{-1})
F_j	Volumetric flow rate of stream j (L h^{-1})
I_{ap}	Applied current (A); $I(x, t)$ current density (A m^{-2})
J_i^j	Molar flux of species i in domain $j \in \{\text{ano, cat, mb}\}$ ($\text{mol m}^{-2} \text{s}^{-1}$)
$K_{\text{wat,eq}}$	Water autoionization equilibrium constant
k_a	Water-association rate constant ($\text{L mol}^{-1} \text{s}^{-1}$)
k_f, k_r	Forward/reverse complexation rate constants ($\text{L mol}^{-1} \text{s}^{-1}; \text{s}^{-1}$)
k_{int}	Interfacial mass-transfer coefficient (m s^{-1})
L	Membrane thickness (m)
$\mathcal{N}_i$	Total molar transfer rate across the membrane (mol s^{-1})
n_{hyd}	Lithium hydration number (—)
$Q_w^{\text{ano}}, Q_r^{\text{cat}}$	Electro-osmotic/reduction water volumetric rate (L s^{-1})
R	Universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
R_i, R_{assoc}	Homogeneous reaction rate; association rate (M s^{-1})
$r_{\text{OH,prod}}$	Cathodic hydroxide production rate (mol s^{-1})
S	Bulk gradient of the potential (V m^{-1})
T	Absolute temperature (K)
t, x	Time (s); spatial coordinate (m)
u_i^{eff}	Effective ionic mobility, D_i^{eff}/RT
$V_{\text{ano}}, V_{\text{cat}}$	Anode/cathode liquid volume (L)
z_i	Charge number of species i (—)

Greek symbols

$\Delta\Phi_D^j$	Interfacial Donnan potential jump (V)
ϵ	Membrane porosity (—); $\epsilon_0, \epsilon^{\text{mb}}$ permittivities
η	Current efficiency (%)

θ	Characteristic diffusion time, $L^2/D_{\text{Li}}^{\text{eff}}$ (s)
κ^{mb}	Local ionic conductivity (S m^{-1})
λ	Characteristic decay length (m)
ν_w	Water-consumption coefficient (—)
σ_{mb}	Effective ionic conductivity (S m^{-1})
τ_k	Characteristic time of process k (s); τ membrane tortuosity (—)
Φ, Φ^{mb}	Electric potential (V)

Superscripts/Subscripts

ano, cat, mb	Anode, cathode, membrane
rec, fresh	Recycled, fresh feed
eff	Effective (membrane-corrected) property
ap, int, prod	Applied, interfacial, production
*	Dimensionless quantity

Appendix A. Dimensionless Model Formulation

The governing equations are non-dimensionalized using the characteristic length L (membrane thickness) and the diffusion time scale of lithium ions, defined by the following scaling relations:

$$x = Lx^*, \quad t = \frac{L^2}{D_{\text{Li}}^{\text{eff}}} t^* \quad (\text{A1})$$

where $x^* \in [0, 1]$ and t^* represent the dimensionless position and time, respectively.

Appendix A.1. Anode Chamber Balances

The dimensionless mass balances for the anode chamber are given by

$$\frac{dC_{\text{Li}}^{\text{ano}}(t^*)}{dt^*} = \frac{L^2}{D_{\text{Li}}^{\text{eff}} V_{\text{ano}}} \left[\sum_{i \in \{\text{rec, fresh}\}} F_i (C_{\text{Li}}^i - C_{\text{Li}}^{\text{ano}}(t^*)) - Q_w^{\text{ano}}(t^*) C_{\text{Li}}^{\text{ano}}(t^*) - F_{\text{wat}}^{\text{ano}}(t) C_{\text{Li}}^{\text{ano}}(t^*) \right] - \frac{AL}{V_{\text{ano}}} \mathcal{J}_{\text{Li}}^*(0, t^*) \quad (\text{A2a})$$

$$\frac{dC_{\text{OH}}^{\text{ano}}(t^*)}{dt^*} = - \frac{L^2 k_a}{D_{\text{Li}}^{\text{eff}}} \left(C_{\text{H}}^{\text{ano}}(t^*) C_{\text{OH}}^{\text{ano}}(t^*) - \frac{C_{\text{H}_2\text{O}}(t^*)}{K_{\text{wat,eq}}} \right) + \frac{AL}{V_{\text{ano}}} \frac{D_{\text{OH}}^{\text{eff}}}{D_{\text{Li}}^{\text{eff}}} \mathcal{J}_{\text{OH}}^*(0, t^*) - \frac{L^2}{D_{\text{Li}}^{\text{eff}} V_{\text{ano}}} F_{\text{wat}}^{\text{ano}}(t) C_{\text{OH}}^{\text{ano}}(t^*) - \frac{L^2 Q_w^{\text{ano}}(t^*)}{D_{\text{Li}}^{\text{eff}} V_{\text{ano}}} C_{\text{OH}}^{\text{ano}}(t^*) \quad (\text{A2b})$$

The dimensionless interfacial molar fluxes $\mathcal{J}_j^*$ are evaluated using the scaled Nernst–Planck relation:

$$\mathcal{J}_j^*(x^*, t^*) = - \frac{\partial C_j^{\text{mb}}(x^*, t^*)}{\partial x^*} - z_j C_j^{\text{mb}}(x^*, t^*) \frac{\partial \Phi(x^*, t^*)}{\partial x^*} \quad (\text{A3})$$

Appendix A.2. Cathode Chamber Balances

The dimensionless balances for the cathode chamber, accounting for chemical association and water reduction, are

$$\frac{dC_{\text{Li}}^{\text{cat}}(t^*)}{dt^*} = \frac{L^2 F_{\text{Li-OH}}^{\text{rec}}}{D_{\text{Li}}^{\text{eff}} V_{\text{cat}}} (C_{\text{Li-OH}}^{\text{rec}} - C_{\text{Li}}^{\text{cat}}(t^*)) + \frac{AL}{V_{\text{cat}}} \mathcal{J}_{\text{Li}}^*(1, t^*) - \mathcal{R}_{\text{flow}}^*(t^*) C_{\text{Li}}^{\text{cat}}(t^*) - \frac{L^2}{D_{\text{Li}}^{\text{eff}}} R_{\text{assoc}}(t^*), \quad (\text{A4a})$$

$$\frac{dC_{OH}^{cat}(t^*)}{dt^*} = \frac{L^2 F_{Li-OH}^{rec}}{D_{Li}^{eff} V_{cat}} (C_{Li-OH}^{rec} - C_{OH}^{cat}(t^*)) + \frac{L^2 r_{OH,prod}(t^*)}{D_{Li}^{eff} V_{cat}} + \frac{AL}{V_{cat}} \frac{D_{OH}^{eff}}{D_{Li}^{eff}} \mathcal{J}_{OH}^*(1, t^*) - \mathcal{R}_{flow}^*(t^*) C_{OH}^{cat}(t^*) - \frac{L^2}{D_{Li}^{eff}} R_{assoc}(t^*), \quad (A4b)$$

$$\frac{dC_{Li-OH}^{cat}(t^*)}{dt^*} = -\frac{L^2 F_{Li-OH}^{rec}}{D_{Li}^{eff} V_{cat}} C_{Li-OH}^{cat}(t^*) + \frac{L^2}{D_{Li}^{eff}} R_{assoc}(t^*) - \mathcal{R}_{flow}^*(t^*) C_{Li-OH}^{cat}(t^*) \quad (A4c)$$

where $\mathcal{R}_{flow}^*(t^*) = \frac{L^2(Q_w^{cat}(t^*) - Q_r^{cat}(t^*))}{D_{Li}^{eff} V_{cat}}$. The water reduction term is

$$Q_r^{cat}(t^*) = \frac{\nu_w I_{ap}(t^*)}{F C_{H_2O}} \quad (A5)$$

Appendix A.3. Membrane PDEs

The dimensionless governing equations for transport within the membrane ($x^* \in [0, 1]$) are

$$\frac{\partial C_{Li}^{mb}(x^*, t^*)}{\partial t^*} = \frac{\partial}{\partial x^*} \left[\frac{\partial C_{Li}^{mb}(x^*, t^*)}{\partial x^*} + z_{Li} C_{Li}^{mb}(x^*, t^*) \frac{\partial \Phi(x^*, t^*)}{\partial x^*} \right] \quad (A6a)$$

$$\frac{\partial C_{OH}^{mb}(x^*, t^*)}{\partial t^*} = \frac{D_{OH}^{eff}}{D_{Li}^{eff}} \frac{\partial}{\partial x^*} \left[\frac{\partial C_{OH}^{mb}(x^*, t^*)}{\partial x^*} + z_{OH} C_{OH}^{mb}(x^*, t^*) \frac{\partial \Phi(x^*, t^*)}{\partial x^*} \right] \quad (A6b)$$

The dimensionless flux $\mathcal{J}_i^*(x^*, t^*)$ is defined such that $J_i^{mb}(x, t) = \frac{D_i^{eff}}{L} \mathcal{J}_i^*(x^*, t^*)$:

$$\mathcal{J}_i^*(x^*, t^*) = - \left(\frac{\partial C_i^{mb}(x^*, t^*)}{\partial x^*} + z_i C_i^{mb}(x^*, t^*) \frac{\partial \Phi(x^*, t^*)}{\partial x^*} \right) \quad (A7)$$

Appendix A.4. Dimensionless Boundary Conditions

The boundary conditions are simplified by grouping the mass transfer and diffusion terms into a single coefficient ratio:

$$\mathcal{J}_{Li}^*(0, t^*) = \frac{k_{int} L}{D_{Li}^{eff}} (C_{Li}^{ano}(t^*) - C_{Li}^{mb}(0, t^*)) \quad (A8a)$$

$$\mathcal{J}_{OH}^*(0, t^*) = \frac{k_{int} L}{D_{OH}^{eff}} (C_{OH}^{mb}(0, t^*) - C_{OH}^{ano}(t^*)) \quad (A8b)$$

$$\mathcal{J}_{Li}^*(1, t^*) = \frac{k_{int} L}{D_{Li}^{eff}} (C_{Li}^{mb}(1, t^*) - C_{Li}^{cat}(t^*)) \quad (A8c)$$

$$\mathcal{J}_{OH}^*(1, t^*) = \frac{k_{int} L}{D_{OH}^{eff}} (C_{OH}^{cat}(t^*) - C_{OH}^{mb}(1, t^*)) \quad (A8d)$$

Appendix A.5. Potential Distribution

The dimensionless potential distribution and its gradient $\mathcal{S}$ are governed by the following equations, which maintain explicit dependence on the dimensionless spatial coordinate x^* and time t^* :

$$\frac{\partial \Phi(x^*, t^*)}{\partial x^*} = \mathcal{S}(x^*, t^*) = - \frac{I(x^*, t^*) + \sum_i z_i \left(\frac{D_i^{eff}}{D_{Li}^{eff}} \right) \frac{\partial C_i(x^*, t^*)}{\partial x^*}}{\sum_i z_i^2 \left(\frac{D_i^{eff}}{D_{Li}^{eff}} \right) C_i(x^*, t^*)}, \quad (A9a)$$

$$\frac{\partial^2 \Phi(x^*, t^*)}{\partial (x^*)^2} = \frac{\partial \mathcal{S}(x^*, t^*)}{\partial x^*} = -\frac{1}{\kappa^{\text{mb}}(x^*, t^*)} \left[\sum_i z_i \left(\frac{D_i^{\text{eff}}}{D_{\text{Li}}^{\text{eff}}} \right) \frac{\partial^2 C_i(x^*, t^*)}{\partial (x^*)^2} + \mathcal{S}(x^*, t^*) \frac{\partial \kappa^{\text{mb}}(x^*, t^*)}{\partial x^*} \right] \quad (\text{A9b})$$

where the dimensionless local ionic conductivity and its spatial gradient are defined as

$$\kappa^{\text{mb}}(x^*, t^*) = \sum_i z_i^2 \left(\frac{D_i^{\text{eff}}}{D_{\text{Li}}^{\text{eff}}} \right) C_i(x^*, t^*) \quad (\text{A10a})$$

$$\frac{\partial \kappa^{\text{mb}}(x^*, t^*)}{\partial x^*} = \sum_i z_i^2 \left(\frac{D_i^{\text{eff}}}{D_{\text{Li}}^{\text{eff}}} \right) \frac{\partial C_i(x^*, t^*)}{\partial x^*} \quad (\text{A10b})$$

Appendix B. Local Electric Field Formulation

This appendix collects the dimensional expressions for the bulk electric-field gradient used in Section 2.2.4 [Equation (6)], omitted from the main text for readability. In the migration-dominant regime, the bulk gradient $\mathcal{S}(x, t) \equiv \partial \Phi^{\text{mb}} / \partial x$ is obtained by rearranging the total current density $I(x, t) = F \sum_i z_i J_i(x, t)$ and applying the Nernst–Einstein relation ($u_i^{\text{eff}} = D_i^{\text{eff}} / RT$):

$$\mathcal{S}(x, t) = -RT \frac{I(x, t) + F \sum_i z_i D_i^{\text{eff}} \partial C_i^{\text{mb}}(x, t) / \partial x}{F^2 \sum_i z_i^2 D_i^{\text{eff}} C_i^{\text{mb}}(x, t)}. \quad (\text{A11})$$

This keeps the field self-consistently coupled to the local concentrations, capturing the non-uniform conductivity and diffusion potentials of the membrane. Because the total current density is spatially invariant ($\partial I / \partial x = 0$), the curvature of the field follows by differentiation:

$$\frac{\partial \mathcal{S}(x, t)}{\partial x} = -\frac{1}{\kappa^{\text{mb}}(x, t)} \left[F \sum_i z_i D_i^{\text{eff}} \frac{\partial^2 C_i^{\text{mb}}(x, t)}{\partial x^2} + \mathcal{S}(x, t) \frac{\partial \kappa^{\text{mb}}(x, t)}{\partial x} \right], \quad (\text{A12})$$

where the local ionic conductivity and its spatial gradient are

$$\kappa^{\text{mb}}(x, t) = \frac{F^2}{RT} \sum_i z_i^2 D_i^{\text{eff}} C_i^{\text{mb}}(x, t), \quad \frac{\partial \kappa^{\text{mb}}(x, t)}{\partial x} = \frac{F^2}{RT} \sum_i z_i^2 D_i^{\text{eff}} \frac{\partial C_i^{\text{mb}}(x, t)}{\partial x}. \quad (\text{A13})$$

Nomenclature (Appendix B)

Symbol	Description	Unit
$\mathcal{S}(x, t)$	Bulk gradient of the membrane potential, $\partial \Phi^{\text{mb}} / \partial x$	V m^{-1}
$\Phi^{\text{mb}}(x, t)$	Electric potential in the membrane	V
$I(x, t)$	Total current density	A m^{-2}
$\kappa^{\text{mb}}(x, t)$	Local ionic conductivity of the membrane	S m^{-1}
u_i^{eff}	Effective ionic mobility, D_i^{eff} / RT	mol s kg^{-1}
D_i^{eff}	Effective diffusion coefficient of species i	$\text{m}^2 \text{s}^{-1}$
$C_i^{\text{mb}}(x, t)$	Membrane concentration of species i	M
z_i	Charge number of species i	—
F	Faraday constant	C mol^{-1}
R	Universal gas constant	$\text{J mol}^{-1} \text{K}^{-1}$
T	Absolute temperature	K
x, t	Spatial coordinate; time	m; s

Appendix C. Membrane Fluxes, Boundary Conditions, and Auxiliary Cathodic Rates

This appendix collects the supporting transport and kinetic expressions referenced in Sections 2.2.2–2.2.3, relocated from the main text for readability. It gathers the general Nernst–Planck membrane flux, the interfacial (Robin) boundary conditions, and the auxiliary cathodic water-consumption and association-rate definitions.

Appendix C.1. Nernst–Planck Membrane Flux

The molar flux of species $i \in \{\text{Li}^+, \text{OH}^-\}$ within the membrane, combining diffusion and electromigration, is

$$J_i^{\text{mb}}(x, t) = -D_i^{\text{eff}} \left(\frac{\partial C_i^{\text{mb}}(x, t)}{\partial x} + \frac{z_i F}{RT} C_i^{\text{mb}}(x, t) \frac{\partial \Phi^{\text{mb}}(x, t)}{\partial x} \right). \quad (\text{A14})$$

The interfacial fluxes used in the chamber balances are (A14) evaluated at the domain boundaries, i.e., $J_i^{\text{ano}}(t) \equiv J_i^{\text{mb}}(0, t)$ at the anode ($x = 0$) and $J_i^{\text{mb}}(L, t)$ at the cathode ($x = L$).

Appendix C.2. Interfacial (Robin) Boundary Conditions

Mass transfer at the membrane faces couples the boundary fluxes to the time-dependent chamber concentrations $C_i^{\text{ano}}(t)$ and $C_i^{\text{cat}}(t)$ through the interfacial mass-transfer coefficient k_{int} , which is assumed equal for both ions and both faces:

$$J_{\text{Li}}^{\text{mb}}(0, t) = k_{\text{int}} \left(C_{\text{Li}}^{\text{ano}}(t) - C_{\text{Li}}^{\text{mb}}(0, t) \right), \quad (\text{A15a})$$

$$J_{\text{OH}}^{\text{mb}}(0, t) = k_{\text{int}} \left(C_{\text{OH}}^{\text{mb}}(0, t) - C_{\text{OH}}^{\text{ano}}(t) \right), \quad (\text{A15b})$$

$$J_{\text{Li}}^{\text{mb}}(L, t) = k_{\text{int}} \left(C_{\text{Li}}^{\text{mb}}(L, t) - C_{\text{Li}}^{\text{cat}}(t) \right), \quad (\text{A15c})$$

$$J_{\text{OH}}^{\text{mb}}(L, t) = k_{\text{int}} \left(C_{\text{OH}}^{\text{cat}}(t) - C_{\text{OH}}^{\text{mb}}(L, t) \right). \quad (\text{A15d})$$

Appendix C.3. Auxiliary Cathodic Rates

Local water consumption by the cathodic reduction and the lithium–hydroxide association rate entering the cathode balances are

$$Q_r^{\text{cat}}(t) = \frac{\nu_w I_{\text{ap}}(t)}{F C_{\text{H}_2\text{O}}}, \quad (\text{A16})$$

$$R_{\text{assoc}}(t) = k_f C_{\text{Li}}^{\text{cat}}(t) C_{\text{OH}}^{\text{cat}}(t) - k_r C_{\text{LiOH}}^{\text{cat}}(t), \quad (\text{A17})$$

where $\nu_w = 1.0$ (mol H_2O per mol e^-) is the water-consumption coefficient of the cathodic reduction, consistent with the 1 : 1 stoichiometry between consumed water and produced hydroxide.

Appendix C.4. Nomenclature (Appendix C)

Symbol	Description	Unit
$J_i^{\text{mb}}(x, t)$	Molar flux of species i in the membrane	$\text{mol m}^{-2} \text{s}^{-1}$
D_i^{eff}	Effective diffusion coefficient of species i	$\text{m}^2 \text{s}^{-1}$
$C_i^{\text{mb}}(x, t)$	Membrane concentration of species i	M
$C_i^{\text{ano}}, C_i^{\text{cat}}$	Anode/cathode bulk concentration of species i	M
$C_{\text{LiOH}}^{\text{cat}}$	Cathode concentration of the LiOH complex	M
$C_{\text{H}_2\text{O}}$	Molar concentration of water	M
z_i	Charge number of species i	—
$\Phi^{\text{mb}}(x, t)$	Electric potential in the membrane	V
k_{int}	Interfacial mass-transfer coefficient	m s^{-1}
$Q_r^{\text{cat}}(t)$	Volumetric water-consumption rate (cathode)	L s^{-1}
$R_{\text{assoc}}(t)$	Lithium–hydroxide association rate	M s^{-1}
k_f, k_r	Forward/reverse complexation rate constants	$\text{L mol}^{-1} \text{s}^{-1}, \text{s}^{-1}$
$I_{\text{ap}}(t)$	Applied current	A
v_w	Water-consumption coefficient of the reduction	—
F	Faraday constant	C mol^{-1}
R	Universal gas constant	$\text{J mol}^{-1} \text{K}^{-1}$
T	Absolute temperature	K
x, t	Spatial coordinate; time	m; s

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