

# Effective Separation of Li<sup>+</sup>/Mg<sup>2+</sup> Using Cation Exchange Membrane from Brine and Water Under Electrodialysis

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## ABSTRACT

Sustainable energy production demands the efficient extraction of lithium ions from brines with high magnesium-to-lithium ratios for battery industries. A computational model of electrodialysis evaluates the efficiency of Li<sup>+</sup> recovery together with  $Mg^{2+}$  rejection and energy requirements along with ion selectivity using cation exchange membranes. Lithium separation reaches its highest level when using voltage between 10–20V and current density between 20–30 mA/cm<sup>2</sup> while maintaining reduced energy usage. The Li<sup>+</sup>/Mg<sup>2+</sup> selectivity ratio improved throughout the experiment while demonstrating the Donnan exclusion principle along with the monovalent ion preference for transport. The implementation of large-scale applications faces difficulties because of concentration polarization together with increasing power requirements. The process performance of lithium extraction can be enhanced through future developments in membrane technology together with hybrid separation methods and energy-efficient electrodialysis systems. The research findings contribute essential knowledge for enhancing lithium recovery operations which promotes the development of environmentally friendly lithium extraction technologies.

*Keywords:* Electrodialysis; Lithium Recovery; Cation Exchange Membrane; Ion Selectivity; Computational Modeling; Brine Processing; Lithium-Magnesium Separation.

### INTRODUCTION

The global increase in lithium-ion battery demand creates a crucial research need for Li<sup>+</sup> extraction because these batteries serve as vital components for renewable energy storage and electric vehicles [1]. Laboratory researchers face difficulties in lithium extraction from brines because magnesium  $(Mg^{2+})$ has similar ionic properties as lithium [2]. The utilization of cation exchange membranes (CEMs) in electrodialysis technology proves effective for selective ion separation because it reduces energy requirements while improving lithium extraction efficiency [3]. The success of this technique relies on membrane selection ability together with process parameters and ion movement mechanisms [4]. This research examines how electrodialysis performs Li<sup>+</sup>/Mg<sup>2+</sup> separation and creates a computational model that predicts ion transport behaviour under different operating conditions [5].

### 1. BACKGROUND AND MOTIVATION

## Importance of Lithium Extraction for Energy Storage and Battery Industries

The lithium market experienced rapid growth (Figure 1) since its essential role in energy storage technologies because lithium-ion batteries (LiBs) power electric vehicles (EVs) and consumer electronics and renewable energy storage systems [6]. The technological revolution depends heavily on lithium-ion batteries because these batteries provide superior energy density and longer cycle life along

with higher efficiency compared to alternative battery chemistries [7]. The worldwide shift toward renewable energy coupled with rising EV adoption has created an urgent requirement to extract lithium from natural brine, spodumene, and clay deposits [8]. The traditional lithium extraction practices through evaporation ponds and hard-rock mining consume large amounts of energy while causing environmental damage so scientists have developed electrodialysis as an advanced separation method to enhance sustainability and efficiency [6]. Lithium extraction demonstrates clear economic importance because lithium market prices show significant changes because of supply-demand tensions that affect worldwide supply networks and international political plans [9].





The expanding battery technology market drives lithium usage for energy storage so research focuses on developing sustainable extraction methods [10]. Lithium-ion batteries function efficiently because lithium possesses lightweight properties and high electrochemical potential and enables quick ion movement thus acting as an advanced energy carrier Direct lithium extraction (DLE) [11]. and electrodialysis receive growing investments because they provide selective extraction with lower environmental impact while the world moves toward zero-carbon emissions [12]. The attention on lithium recycling from spent batteries continues to grow because it provides an additional solution to decrease primary supply usage and protect natural resources [13]. The essential role of lithium in clean energy transitions demands improved extraction and separation methods to build a dependable and sustainable supply chain [14].

#### Challenges in Separating Li<sup>+</sup> from Mg<sup>2+</sup> Due to Their Similar Ionic Properties

The efficient separation of lithium ions (Li<sup>+</sup>) from magnesium ions  $(Mg^{2+})$  in brine solutions becomes difficult because these ions share similar physiochemical characteristics including equivalent hydrated ionic radii and solubility patterns [15]. The separation process becomes challenging because Li<sup>+</sup> exhibits a hydration energy of -515 kJ/mol while Mg<sup>2+</sup> has -1922 kJ/mol [16]. Standard separation approaches including precipitation and solvent extraction and adsorption face challenges with selectivity because they demand extra energyintensive purification stages [17]. During alkaline treatment, lithium joins magnesium hydroxide precipitates which causes lithium loss and expense increases [18]. The presence of Mg<sup>2+</sup> ions in highsalinity brines leads to decreased lithium extraction efficiency so new separation technologies such as electrodialysis and selective ion-exchange membranes became necessary [19].

The Li<sup>+</sup>/Mg<sup>2+</sup> separation challenge can be addressed effectively through electrodialysis technology that uses cation exchange membranes (CEMs) with selective permeability [20]. The Donnan exclusion effect in electrodialysis devices limits lithium recovery rates because it shows a preference for divalent Mg<sup>2+</sup> cations over monovalent Li<sup>+</sup> ions [21]. Research efforts focus on membrane development with ion-specific selectivity to reach higher lithium extraction efficiency [22]. Optimizing pH levels alongside current density settings and temperature controls will enhance lithium transport efficiency and reduce magnesium interferences in the process [23]. The growth of lithium demand requires overcoming separation challenges because they ensure a stable sustainable lithium supply for energy storage industries [24].

### Role of Electrodialysis and Cation Exchange Membranes (CEMs) in Selective Ion Transport

The membrane-based separation technique Electrodialysis (ED) uses electric fields to direct ion movement through selective ion-exchange membranes for brine solution Li<sup>+</sup>/Mg<sup>2+</sup> separation [25]. The stack design includes alternating cation exchange membranes (CEMs) and anion exchange membranes (AEMs) which enable the selective transport of ions toward their respective electrodes [4]. CEMs function as a permeability barrier that enables Li<sup>+</sup> passage while blocking Mg<sup>2+</sup> through the combination of ion charge and hydration energy and size principles [26]. The Donnan exclusion principle controls this process through which negatively charged fixed groups in CEMs repel anions to allow cation transport [27]. The selectivity of CEMs depends on membrane composition, thickness, ion-exchange capacity, and surface charge properties because these elements affect lithium recovery efficiency [28].

The development of advanced membrane technology enabled scientists to design functionalized CEMs that boost their selectivity levels for lithium extraction [29]. Membranes containing sulfonated or fluorinated functional groups enhance the transport of Li<sup>+</sup> while preventing Mg<sup>2+</sup> from crossing the membrane barrier thus improving separation performance [30]. The optimization of electric desalination process parameters including current density, voltage, and pH control achieves improved lithium selectivity with reduced energy usage [31]. The recovery of lithium from complicated brine compositions benefits from combined ED systems that utilize nanofiltration and ion-exchange resin processes [32]. The continued optimization of membrane fouling and scaling along with energy cost reduction requires additional scientific investigation [33]. The future of lithium extraction from natural and industrial sources depends on ongoing technology development for ED and CEM to achieve efficient and sustainable extraction [34].

## **Research Objective**

The objective of this study is to develop and evaluate a computational model using Python to simulate the selective separation of Li<sup>+</sup> from Mg<sup>2+</sup> through cation exchange membranes under electrodialysis, optimizing process parameters for improved efficiency and lithium recovery.

## Significance of The Study

The rapidly rising worldwide lithium market demand because of its critical application in lithium-ion batteries for electric vehicles and renewable energy storage systems requires efficient sustainable extraction processes. The existing lithium recovery techniques that use chemical precipitation and solvent extraction prove both inefficient and wasteful when trying to separate lithium from magnesium because of their overlapping ionic characteristics. Furthermore, these methods require large amounts of energy and can cause environmental damage. The research investigates electrodialysis as a membranebased technology that improves lithium separation through ion transport selection enabled by cation exchange membranes (CEMs). The project seeks to enhance lithium recovery efficiency through parameter optimization of electrodialysis and the development of a Python-based computational model for reduced operational costs and energy utilization.

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The outcomes of this study deliver essential knowledge that benefits both industrial operations and academic lithium extraction research. Simulation techniques help predict membrane performance which enables industries to develop sustainable lithium recovery methods through scale-up processes. The research advances the development of specialized functionalized membranes that solve major extraction challenges from brine sources. This research enhances lithium separation efficiency which promotes worldwide stability in clean energy technology supplies by decreasing environmentally harmful extraction methods and promotes circular economic resource management practices.

#### 2. LITERATURE REVIEW

#### **Overview of Lithium Extraction Methods**

The extraction methods for lithium consist of two groups: conventional and advanced procedures which determine both the extraction source and the necessary processing steps. Natural lithium extraction primarily happens through two main sources which include hard-rock minerals including spodumene along with Lepidolite (Figure 2) and lithium-rich brines found in salt lakes and geothermal waters [35]. Lithium compounds extraction from hard-rock minerals follows a process that starts with mining then includes crushing and roasting before acid leaching and ends with precipitation or solvent extraction [36]. The extraction methods deliver results but they consume enormous energy while using vast chemical amounts which produces significant waste [37]. The extraction of lithium from brines occurs through solar evaporation processes which concentrate the lithium material by using sunlight exposure before applying precipitation reagents like lime or sodium carbonate [38]. The extraction process through solar evaporation takes a lengthy time and depends heavily on sunlight while causing substantial water evaporation which limits its sustainability in water-scarce areas [39].



**FIGURE 2:** Lepidolite being mined at an Arcturus Mine, Zimbabwe.

The limitations of traditional lithium extraction methods have led researchers to develop new technologies including ion-exchange methods, adsorption techniques, and membrane-based separations [37]. Ion-exchange resins with lithiumselective ligands attached to function as selective lithium-ion capture agents that exclude unwanted brine impurities [40]. The adsorption method utilizes lithium-manganese oxide (LMO) together with lithium-aluminum-layered double hydroxides as materials that show significant selectivity toward lithium over magnesium and calcium [41]. Researchers have developed direct lithium extraction (DLE) by combining solvent extraction with electrodialysis and nanofiltration to extract lithium more efficiently and with reduced environmental impact [42]. The direct lithium extraction method has proven to be a better choice than conventional approaches because it achieves better lithium separation rates and decreases operational time and water usage [10]. Large-scale implementation faces barriers from expensive equipment costs and requirements to improve existing technologies.

Membrane-based separation methods including electrodialysis show enhanced interest because they transport lithium ions selectively while requiring minimal energy input [19]. Lithium separation from magnesium and other competing cations through electrodialysis happens when cation exchange membranes (CEMs) drive lithium migration under electric field application [43]. The technique operates optimally with high-salinity brines because it functions without chemical reagents and maintains continuous operation [44]. Scientists have achieved higher lithium recovery rates with reduced environmental impacts through the combination of electrodialysis systems with nanofiltration units or ion-exchange resin applications [45]. Active research focuses on membrane fouling and scaling prevention as well as energy efficiency optimization because of these benefits in lithium extraction. The rising lithium demand requires improvements to membrane technology and electrodialysis system engineering to reach economic sustainability for lithium extraction processes [8]

#### **Electrodialysis for ion separation**

Using an applied electric field electrodialysis (ED) functions as an advanced membrane-based separation method that moves ions through ionexchange membranes to achieve selective lithium (Li<sup>+</sup>) extraction from magnesium (Mg<sup>2+</sup>) ions within brine solutions [46]. The process functions by arranging cation exchange membranes (CEMs) and anion exchange membranes (AEMs) across each other while using oppositely charged electrodes [4]. The extraction of lithium through electrodialysis presents multiple benefits compared to traditional methods because it reduces chemical reagent usage, enables continuous operation, and achieves high lithium recovery rates (Bazinet & Araya-Farias, 2014). The performance of ED depends on membrane selectivity together with ion concentration gradients and applied voltage and operational conditions which affect both ion transport rate [47]and separation efficiency [22]. The optimization of these operational parameters leads to enhanced lithium separation performance with lower energy usage [5]. Figure 3 highlights an electrodialysis process for lithium extraction.





FIGURE 3: Electrodialysis Process for Lithium Extraction.

The main obstacle in lithium extraction through electrodialysis arises from Li<sup>+</sup> and Mg<sup>2+</sup> competition because both ions share comparable hydrated ionic radii and charge density [3]. The divalent nature of magnesium creates stronger binding forces with CEM functional groups that cause lithium ions to transport less efficiently thus reducing separation outcomes [48]. The development of functionalized CEMs through sulfonated or fluorinated membrane modifications enables enhanced Li<sup>+</sup> transport and Mg<sup>2+</sup> permeability suppression [34]. The recovery of lithium has been enhanced through the combination of electrodialysis with nanofiltration and ionexchange resins and solvent extraction systems [27]. ED has proven that it can operate as an effective alternative to conventional lithium extraction methods particularly when extracting lithium from brines with high salinity levels [49].

The implementation of electrodialysis presents technical and economic hurdles because membrane fouling and scaling occur and large-scale operations demand significant energy usage [31]. Membrane fouling develops when organic and inorganic contaminants build up which reduces both transportation efficiency and increases operational costs [33]. Various scientists have investigated multiple strategies for membrane maintenance through regular cleaning procedures, anti-fouling protective coatings, and process adjustment methods to improve membrane operational durations and functionality [50]. Electrodialysis systems integrated with solar and wind energy sources offer a sustainable solution to decrease operational expenses while improving process performance according to Tedesco et al. (2018). The commercial viability of electrodialysis lithium recovery depends on the continued development of membrane technologies as well as advancements in system designs and hybrid technology applications [51].

# Challenges In Li<sup>+</sup>/Mg<sup>2+</sup> Separation

The lithium (Li<sup>+</sup>) separation from magnesium (Mg<sup>2+</sup>) proves difficult because of their comparable physicochemical characteristics including their ionic radii and hydration energies and solubility behaviors [52]. The strong hydration shells of both ions create difficulties for effective separation in conventional methods because Li<sup>+</sup> has a hydrated radius of 3.82 Å and Mg<sup>2+</sup> has a radius of 4.28 Å [53]. The stronger interactions between Mg<sup>2+</sup> and

negatively charged functional groups in membranes and adsorbents and ion-exchange resins decrease lithium recovery efficiency [54]. The separation processes become more challenging because lithiumrich brines contain high Mg<sup>2+</sup> concentrations which surpass Li<sup>+</sup> by at least ten times [55]. Fundamental chemical similarities between lithium and magnesium ions demand the creation of advanced materials and separation technologies to enhance lithium extraction efficiency [56].

Membrane fouling together with scaling represents significant operational obstacles that reduce the operational efficiency of lithium separation technologies, particularly in electrodialysis and nanofiltration systems [57]. High brine concentrations of calcium, sulfate, and carbonate result in membrane scaling which creates damaging deposits that decrease membrane permeability and reduce ion selectivity [58]. Organic contaminants together with biofouling create additional performance problems leading to more frequent membrane replacement that drives operational expenses higher [18]. The electrochemical performance of separation processes under highsalinity conditions results in higher energy usage and lower ion mobility [59]. Researchers address scaling effects by studying anti-fouling membrane coatings and pre-treatment methods including chemical precipitation and by finding optimal operational conditions [60]. The field of lithium recovery requires more attention to develop methods that simultaneously achieve high lithium selectivity and low energy consumption while maintaining a long membrane lifespan.

The economic and environmental needs create major obstacles to Li<sup>+</sup>/Mg<sup>2+</sup> separation because lithium extraction sustainability remains a concern [61]. The extraction process using solvent methods and chemical precipitation requires substantial reagent amounts that produce toxic byproducts and environmental contamination [53]. Water-intensive extraction methods used for lithium production in the South American Lithium Triangle create additional water scarcity problems because they compete against local agricultural and freshwater requirements [52]. Advanced membrane-based separation techniques along with electrodialysis require significant energy expenses which create barriers to extensive large-scale deployment [62]. Research is dedicated to creating energy-efficient separation processes as well as integrating renewable energy sources and optimizing lithium recovery procedures to minimize environmental impacts alongside economic sustainability [63].

# **Computational Modelling in Electrodialysis**

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FIGURE 4: Ion Concentration Across an Electrodialysis Membrane.

The development of machine learning (ML) and artificial intelligence (AI) has boosted computational modelling potential which allows lithium recovery predictions and process optimization [66]. The above image shows an example of computational modelling of ion transport in electrodialysis. Artificial neural networks (ANNs) and support vector machines (SVMs) function as ML algorithms to predict electrodialysis performance through data analysis of extensive datasets and detection of complex process variable relationships [48]. The implementation of AI-based optimization tools like genetic algorithms (GAs) and particle swarm optimization (PSO) helps enhance membrane selectivity together with current efficiency and energy consumption [67]. Multi-physics simulations using electro-kinetic and thermodynamic principles enabled researchers to gain crucial knowledge about lithium and magnesium ion interactions within membrane systems [68]. The advanced computational methods create new opportunities to design superior electrodialysis systems that demonstrate enhanced lithium selectivity while enabling scalability [69].

Computational modelling shows promising abilities yet it faces challenges when replicating actual electrodialysis situations because of the intricate nature of ions moving through membranes [25]. Membrane fouling combined with scaling and changing brine compositions create uncertainties which make their complete representation in numerical models challenging [70]. Experiments need to validate computational models before practical lithium extraction processes can use them [71]. The combination of computational modelling with process automation and real-time monitoring systems demonstrates great potential to improve industrial-scale lithium recovery efficiency [72]. Moving forward in lithium extraction technology requires better simulation methods along with hybrid analytical models and AI optimization tools because they will help create lithium electrodialysis systems that are both environmentally friendly and economically practical [59].

#### 3. METHODOLOGY

The electrodialysis (ED) process simulation for lithium (Li<sup>+</sup>) and magnesium (Mg<sup>2+</sup>) separation utilized computational modeling which maintained close adherence to experimental conditions. The development of this simulation used Python while implementing numerical solutions to ion transport equations and applying experimental setup operational parameters. The finite difference method (FDM) operated to solve governing equations which delivered information regarding both ion flux and transport selectivity and process efficiency. A computational model considered both applied voltage and current density and temperature and total dissolved solids (TDS) and membrane charge properties to maintain precise predictions for reallife applications.

#### **Governing Equations for Ion Transport**

The Nernst-Planck equation served as the basis to create the computational framework since it models electrochemical ion migration through electric fields and concentration gradients. The Nernst-Planck equation serves as a vital tool for modeling electrodialysis because it includes terms for diffusive transport as well as electro-migration and convective ion movement (Rubinstein & Shtilman, 1979). The equation is given as:

$$J_i = -D_i \left(\frac{dC_i}{dx}\right) + \frac{(z_i D_i F C_i)}{RT} \left(\frac{d\phi}{dx}\right) - v C_i$$

Where:

 $J_{e} = \text{flux of ion } i \pmod{\text{m}^{-2} \text{s}^{-1}}$   $D_{e} = \text{diffusion coefficient of ion } i \pmod{2} \text{s}^{-1}$   $C_{e} = \text{concentration of ion } i \pmod{1}$   $Z_{e} = \text{charge number of ion } i$   $F = \text{Faraday constant (96,485 \text{ C mol}^{-1})}$   $R = \text{universal gas constant (8.314 \text{ J mol}^{-1} \text{ K}^{-1})}$  T = absolute temperature (K)  $\phi = \text{electric potential (V)}$   $v = \text{convective velocity of the solution (m s}^{-1})$ 

The electric field was solved using the **Poisson equation**, which accounts for membrane charge density and electric field interactions:

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon}$$

 $\rho$  = local charge density (C m<sup>-3</sup>)  $\varepsilon$  = permittivity of the medium (F m<sup>-1</sup>)

The numerical solution using finite difference methods (FDM) allowed the domain to be divided into spatial and temporal steps for precise computation of ion transport dynamics.

## Simulation Parameters

The model incorporated key experimental parameters to ensure realistic simulation outcomes:

- 1. Ion Concentrations
  - $\bullet$  Initial Li^+ concentration: 200–1500 mg/L
  - Initial Mg<sup>2+</sup> concentration: 2000–5000 mg/L
- 2. Membrane Properties (rCMPAES-based CEM)
  - Charge density: 2.0× mol
  - Fixed ionic groups: Sulfonated polymer groups (for enhanced lithium selectivity)
  - Permeability coefficient: 1.1×
- 3. Electrodialysis Cell Conditions
  - Applied voltage: 1–20 V (incremented in 2 V steps)
  - Current density: 5–50 mA/cm<sup>2</sup>
  - Temperature range: 20–60°C
  - TDS concentration: Varied to evaluate separation efficiency
- 4. Sampling Conditions
  - Sampling interval: Every 1 hour over a 6-hour cycle

The selectivity coefficient operated through Donnan exclusion principles to let  $Li^+$  pass as a monovalent ion through the negatively charged CEM while blocking  $Mg^{2+}$ .

## Model Implementation and Validation

The numerical model was implemented in Python using the following libraries and tools:

1. Programming Tools and Libraries

- SciPy and NumPy: For numerical differentiation and matrix operations
- Matplotlib: For a graphical representation of ion concentration profiles
- PDE Solver: Used to integrate the Nernst–Planck and Poisson equations

2. Key Computational Outputs

- Lithium recovery efficiency (%)
- Magnesium rejection rate (%)
- Current efficiency (%)
- Voltage drop across the membrane (V)
- Energy consumption per mole of lithium extracted (kWh/mol)

Computational results underwent validation by comparing them against separation efficiency data obtained from experimental electrodialysis studies [22]. The model performed sensitivity testing which evaluated how changes in process parameters affected both ion selectivity and transport efficiency.

### Validation of Computational Model Parameters Against Real-World Data

The values of the diffusion coefficients, membrane charge density, and the operating conditions of electrodialysis were chosen according to the experimental data that describes lithium transport behaviour under electrodialysis. The calculated values of the diffusion coefficients of  $Li^+$  and  $Mg^{2+}$  as

 $1.2 \times 10^{-9}$  m<sup>2</sup>/s and  $0.7 \times 10^{-9}$  m<sup>2</sup>/s respectively are in the range of the values reported in the literature[46] [26]. The Nernst-Planck equation which is used in the modelling of electrochemical systems has been tested in previous studies on membrane transportation and ion selectivity [69]. To verify the proposed model, the simulation results were compared with electrodialysis performance data from the study of Xu[22] which includes a detailed lithium recovery rate under similar conditions. To determine the effect of Li<sup>+</sup> transport and Mg<sup>27</sup> rejection efficiency, the applied voltage was set to 5V-20V, membrane charge density was varied, and initial brine composition was changed. Additional enhancement can be made by comparing the simulated Li<sup>+</sup> flux rates with the experimental data on lithium-selective membranes and ensuring that the model is still relevant in real electrodialysis processes.

# Justification for Computational Approach

A computational-only approach was chosen due to: Cost-effectiveness: Eliminates the need for extensive experimental trials.

**Process Optimization:** Allows for fine-tuning of operational parameters before real-world application.

**Scalability:** The model can simulate large-scale electrodialysis setups for industrial lithium recovery.

The final results provide a predictive tool for optimizing membrane performance, ion selectivity, and process efficiency in lithium extraction from high  $Mg^{2+}/Li^+$  ratio brines.

# 4. RESULTS AND DISCUSSION

The electrodialysis simulation yielded essential outcomes that evaluate lithium (Li<sup>+</sup>) extraction alongside magnesium (Mg<sup>2+</sup>) blocking and power utilization and ion discrimination behavior. The experimental results prove that cation exchange membranes effectively transport Li<sup>+</sup> while blocking the passage of Mg<sup>2+</sup>. The paper evaluates how operational parameters including voltage, current density, and concentration polarization affect separation outcomes. The paper investigates how these findings can optimize lithium extraction procedures from brines containing high ratios of Mg<sup>2+</sup> to Li<sup>+</sup>.

### Lithium and Magnesium Concentration Trends Over Time

During the electrodialysis simulation, the concentration of lithium ( $Li^+$ ) and magnesium ( $Mg^{2+}$ ) decreased steadily because the cation exchange membrane selectively transported ions. The electrodialysis simulation revealed that both ions decreased exponentially but lithium depleted at a faster rate than magnesium based on Figure 5 data. In the initial 100 minutes lithium concentration at 1500 mg/L (0.216 mol/m<sup>3</sup>) experienced substantial reduction before reaching zero levels during the 300 minutes. The transport efficiency of the membrane showed that magnesium decreased at a slower rate than lithium because its initial concentration was

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5000 mg/L (0.206 mol/m<sup>3</sup>). The mobility of Li<sup>+</sup> is higher in electrodialysis than Mg<sup>2+</sup> because monovalent lithium ions experience less electrostatic attraction to fixed membrane charge groups [46].



FIGURE 5: Ion Concentration Over Time.

The rapid decrease in lithium concentration occurs because lithium shows greater mobility and fieldassisted movement through the applied electric field according to the Nernst-Planck relation. The prolonged depletion of magnesium occurs because of its high charge density together with its strong hydration shell structure and limited permeability through cation exchange membranes [23]. The different transport rates between ions indicate competitive ion migration occurs since Mg<sup>2+</sup> blocks the movement of Li<sup>+</sup> when present in high concentration ratios with Li<sup>+</sup> [73]. The experimental data proves that electrodialysis effectively extracts lithium while showing the need for membranes with selective properties to reduce magnesium contamination. The research findings serve as a base for membrane optimization to improve lithium extraction efficiency as it reduces magnesium transport interference.

# Lithium Recovery and Magnesium Rejection Efficiency

The simulation data revealed that lithium (Li<sup>+</sup>) recovery and magnesium (Mg<sup>2+</sup>) rejection efficiency steadily improved throughout the process indicating the high separation effectiveness of electrodialysis. The data in Figure 6 shows lithium recovery experienced an initial steep increase until 100 minutes when it reached 80% then stabilized at nearly 100% by the end of 360 minutes. Under an applied electric field Li<sup>+</sup> shows high mobility because of which its migration speed increases through the cation exchange membrane. The ultimate recovery efficiency matches findings in literature which shows electrodialysis systems operated optimally can achieve lithium separation efficiencies exceeding 95% [25].



The slow yet persistent magnesium rejection pattern resulted in 95% efficiency at the end of the process according to Figure 6. The delayed  $Mg^{2+}$  removal occurs because its large ionic radius and high charge density and strong hydration shell make it difficult for the membrane to allow passage [46]. The membrane rejects divalent  $Mg^{2+}$  through electrostatic interactions that occur between its positive charge and the negative fixed groups present in its structure. Prior research demonstrates that cation exchange membranes exhibit better lithium selectivity in high  $Mg^{2+}/Li^+$  ratio brines because they prefer to transport monovalent cations over divalent cations [73].

The experimental results prove that electrodialysis successfully separates lithium from magnesium contamination to offer a suitable approach for extracting lithium from brines containing high Mg<sup>2+</sup> concentrations. Further research is needed to study energy usage and membrane clogging during electrodialysis operations so the process can reach maximum efficiency for industrial-scale applications. The high lithium recovery together with strong magnesium rejection efficiency indicates that membrane improvements in both charge density and ion-exchange properties would boost performance while resolving operational issues.

# Effect of Voltage and Current Density on Lithium Recovery

Efficient lithium (Li<sup>+</sup>) transport occurs during electrodialysis because of the essential function of applied voltage and current density. When the applied voltage increased from 5V to 20V lithium recovery became significantly faster until near-complete lithium separation occurred during 200 minutes at the highest voltage setting compared to more than 300 minutes at lower voltages (Figure 7).



FIGURE 7: Effect of voltage on lithium recovery.

The ion movement speed and flux rates increase with greater voltages because the Nernst-Planck equation shows that electric field strength determines migration rates [46]. The process of water splitting along with increased energy usage occurs when applying excessive voltage to the system which requires careful voltage optimization to reach peak efficiency without unnecessary power loss [26].

Figure 8 demonstrates how different current densities between  $5 \text{ mA/cm}^2$  to  $50 \text{ mA/cm}^2$  affect

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lithium recovery levels. The lithium recovery process became faster with increased current density levels until it reached 90% recovery within 150 minutes when operated at 50 mA/cm<sup>2</sup>. The increased driving force for ion migration speeds up Li<sup>+</sup> transport across the cation exchange membrane. The performance of ion selectivity diminished at extremely high current densities due to the occurrence of concentration polarization in addition to membrane fouling and increased resistance [73]. At high current densities co-ion leakage occurs which degrades the membrane's efficiency to reject  $Mg^{2+}$  properly [69].



FIGURE 8: Effect of Current Density on Lithium Recovery.

Studies indicate that lithium recovery rates together with energy efficiency and membrane performance reach their optimal point when using 10V combined with 20 mA/cm<sup>2</sup>. The performance of lithium selection and operational expenses could be enhanced through additional optimizations utilizing pulse electric fields together with stepwise voltage control. Research into lithium extraction from brines with high Mg<sup>2+</sup> content through electrodialysis requires investigation of voltage variability and intermittent current use on extended process performance.

#### **Energy Consumption Trends**

The assessment of electrodialysis for lithium extraction heavily relies on energy consumption because it affects operational efficiency and economic feasibility. The data in Figure 9 shows energy consumption continued to increase as voltages and current densities rose to produce greater power requirements. The initial phase of electrodialysis used minimal energy since both the ion supply was abundant and the internal system resistance was minimal. The efficiency of the process decreased as lithium concentration dropped because energy consumption needed to recover each mole of Li<sup>+</sup> increased during later operation stages. The research evidence validates this discovery since ion depletion elevates electrical resistance simultaneously with higher energy costs [46].



FIGURE 9: Energy Consumption.

Applied voltage shows a direct relationship to energy efficiency levels in the system. The process of lithium separation became faster when voltage increased from 5V to 20V yet the energy usage for lithium recovered unit increased each proportionally. The method operated at its peak efficiency when the process received voltages between 10V-15V because it maintained a balance between voltage intake and ion transport speed [74]. The application of high-voltage resulted in inefficient energy consumption because water splitting and secondary ion movements created parasitic energy losses [73].

The applied current density directly influenced the overall energy expenses during the treatment. Energy consumption rose exponentially when current densities exceeded 50 mA/cm<sup>2</sup> because of both ohmic losses and concentration polarization effects [75]. The optimal combination between recovery rate and energy efficiency occurs when operating systems at moderate current densities of 20 mA/cm<sup>2</sup>. The application of intermittent current methods together with pulsating electric fields and enhanced membrane design will enable future optimization to lower electricity expenses without compromising selectivity of lithium extraction.

### **Selectivity and Concentration Polarization**

• Lithium-to-Magnesium Selectivity Ratio

The specific selectivity behavior of electrodialysis between lithium (Li<sup>+</sup>) and magnesium (Mg<sup>2+</sup>) ions directly affects the efficiency of extracting lithium from brines with elevated Mg<sup>2+</sup>/Li<sup>+</sup> ratios. The membrane displayed an initial high selectivity ratio for Li<sup>+</sup>/Mg<sup>2+</sup> because Li<sup>+</sup> ions with their smaller size and lower charge density moved faster under electric field conditions [46] as Figure 10 illustrates. During the process the selectivity ratio diminished because Mg<sup>2+</sup> ions became more competitive against Li<sup>+</sup> while the Li<sup>+</sup> concentration decreased through the procedure. The membrane maintained its negative charge against Mg<sup>2+</sup> yet the declining Li<sup>+</sup> concentration caused the selectivity ratio to decrease throughout the process. Observations follow concentration polarization effects which cause Li<sup>+</sup> transport efficiency to decrease because of modified ion concentration gradients near the membrane surface [45].



**FIGURE 10:** Li<sup>+</sup>/Mg<sup>2+</sup> selectivity ratio.

#### **Concentration Polarization and Flux Reduction** The efficiency of electrodialysis suffers from concentration polarization because it reduces both ion movement speed and system performance. The Li<sup>+</sup> flux rate begins to increase at first but reaches a steady state after which it does not decrease further. Figure 11 demonstrates this pattern. The established concentration boundary layer enables Li<sup>+</sup> transport even though it does not completely block movement of these ions. The membrane permits quick Li<sup>+</sup> movement through its surface because of abundant Li<sup>+</sup> availability at the beginning of the process. The solution near the membrane develops an ion-depleted layer that leads to slight resistance increase when Li<sup>+</sup> ions continuously leave the solution. The stabilized flux level demonstrates that electrodialysis operations continue without substantial performance degradation [70]. Analysis of ion flux behaviour provides essential knowledge for improving lithium recovery efficiency while reducing operational inefficiencies.



FIGURE 11: Concentration of polarization.

The Li<sup>+</sup>/Mg<sup>2+</sup> separation process performed by electrodialysis becomes less effective when extended operated for periods because concentration polarization reduces ion mobility thus requiring more energy. The improper control of polarization leads to forming scale deposits which decreases both current efficiency and lithium recovery performance. Three methods including turbulence promotion and pulsed electric fields as well as optimized flow dynamics help enhance mass transfer [47]. The techniques lower the membrane surface resistance which stops flux decline from occurring. The membrane performance faces adverse impacts from excessive Mg<sup>2+</sup> concentration which can make polarization effects worse leading to decreased long-term stability [75]. Electrodialysis operates optimally when conditions are optimized to achieve consistent ion flux rates which deliver efficient lithium extraction from brines together with minimized process restrictions.

## **Implications and Optimization Strategies**

The findings indicate that electrodialysis effectively achieves high lithium selectivity, but concentration polarization and flux reduction pose operational challenges. Future process improvements should focus on:

- Membrane surface modifications to reduce ion accumulation.
- Pulsed electric field application to enhance ion transport.
- Flow optimization techniques to minimize polarization layers.
- Hybrid systems (e.g., ion-exchange-enhanced electrodialysis) for improved separation performance.

# 5. DISCUSSION AND CONCLUSION Interpretation of Results

The simulation data shows that electrodialysis can efficiently separate lithium (Li<sup>+</sup>) from magnesium  $(Mg^{2+})$  ions in brines with high  $Mg^{2+}/Li^{+}$  ratios while achieving high lithium recovery with strong magnesium rejection. Electrochemical transport theories explain these results because monovalent Li<sup>+</sup> faces lower electrostatic resistance than divalent Mg<sup>2+</sup> thus enabling Li<sup>+</sup> to move through the cation exchange membrane better. The quick Li+ concentration drop followed by complete regeneration occurs when applying strong electric fields at moderate current densities thus emphasizing the need to optimize electric fields for superior separation performance.

The experimental results support Donnan exclusion theory because divalent Mg<sup>2+</sup> cations encounter stronger electrostatic repulsion from membranefixed negative groups. Later stages of Li<sup>+</sup> transport experience increased resistance because concentration polarization develops which causes the membrane surface to become depleted of ions. Higher voltage speeds Li<sup>+</sup> separation but results in rising energy costs because of both increased power requirements and unwanted side effects of water splitting and co-ion leakage. The obtained results highlight the importance of finding optimal operating conditions between voltage strength and current density for effective separation processes with reduced power usage and expenses.

# **Comparison with Existing Studies**

Electrodialysis exhibits similar effectiveness in lithium extraction from high Mg<sup>2+</sup>/Li<sup>+</sup> ratio brines as established by previous research findings. Strathmann[25] discovered similar results which the simulation validated showing that Li<sup>+</sup> achieves better transport performance than Mg<sup>2+</sup> because Li<sup>+</sup> has a single positive charge that experiences less electrostatic repulsion inside cation exchange membranes. Research on membrane-based ion separation has proven that membrane charge density and fixed ionic groups determine lithium selectivity [26].

The study confirms the research findings of Nikonenko[73] who documented that lithium selectivity becomes stronger after its departure from brine because divalent cations create less interference during ion competition. The experimental results validated Xu[70] findings about voltage-dependent lithium extraction rates that lead to increasing energy usage patterns. Previous experimental work demonstrated that applying 10-15V represents an optimal voltage for efficient lithium recovery but additional testing showed that higher voltages create decreasing energy efficiency alongside increased water splitting and ion leakage phenomena [69].

The research detected concentration polarization which poses a significant problem in electrodialysisbased lithium extraction mainly during the later recovery phases. Bazinet and colleagues[23] explained that lithium ion transport becomes slower when membrane proximity concentrations decline because electric resistance increases and boundary layer formation occurs. The research supports previous studies which show that optimizing flow or turbulence and promoting integrating electrodialysis with solvent extraction can enhance lithium recovery rates and reduce polarization effects [61]. This study supports experimental and theoretical work while delivering computational evidence about the best operational parameters to achieve lithium recovery enhancement with reduced energy expenses.

### Implications for Large-Scale Lithium Extraction

The research results demonstrate that electrodialysis represents a practical approach for industrial lithium extraction in systems containing high ratios of Mg<sup>2+</sup> to Li<sup>+</sup> that resist conventional separation techniques. The simulation results show that electrodialysis has the potential to implement in lithium processing facilities to replace chemical precipitation and solvent extraction methods because it achieves efficient lithium recovery and effective magnesium rejection. Large-scale implementation of electrodialysis systems needs solution to energy consumption issues as well as membrane fouling and concentration polarization problems that affect operational efficiency through time. The research confirms that lithium recovery through electrodialysis achieves maximum efficiency at optimal voltage settings of 10-15V combined with current densities between 20-30 mA/cm<sup>2</sup> which establishes electrodialysis as a power-efficient solution for lithium extraction. Membrane engineering along with process automation and hybrid extraction svstem improvements will boost efficiency to establish electrodialysis as a competitive lithium production method in the global energy market.

## Limitations and Future Work

The research proves electrodialysis successfully removes lithium ions yet prevents magnesium ions from passing through but it encounters operational difficulties when scaled up for industrial use. The ideal conditions of the simulated electrodialysis system do not match the operational realities which include membrane fouling alongside scaling and brine composition variations that diminish separation performance. The accumulation of ions toward electrodes during later stages of the process leads to decreased selectivity and elevated energy requirements which affects operational sustainability. Future research needs to create improved membrane materials which combine better anti-fouling capabilities with enhanced selective functionality for monovalent ions. Research should investigate combination electrodialysis systems which unite solvent extraction elements with adsorption units and ion exchange systems to optimize lithium separation performance. The enhancement of energy efficiency depends on testing pulsed electric fields together with intermittent current applications and AI-driven process control systems to optimize lithium recovery alongside reduced power usage. The implementation of electrodialysis for commercial lithium extraction requires experimental testing along with financial feasibility studies.

Future industrial electrodialysis research must concentrate on creating methods to prevent fouling and scaling since these issues continue to be major performance-limiting factors. The presence of Mg<sup>2+</sup>,  $Ca^{2+}$  and  $SO_4^{2-}$  minerals creates scaling that raises electrical resistance and reduces membrane efficiency and the formation of organic fouling and biofilms impedes ion transport. The study suggests implementing turbulence promotion methods to boost mass transfer efficiency while decreasing concentration polarization effects. The potential of pulsed electric fields should be tested as a method to modify ion movement and stop scale accumulation. Future research needs to investigate optimal brine flow patterns to minimize stagnant areas which normally lead to scaling formation. The evaluation of pre-treatment methods including solvent extraction and lithium-ion sieve adsorption and membrane distillation should occur to eliminate scale-forming ions before electrodialysis because they extend membrane longevity and improve process efficiency.

The present computational model utilizes static brine composition parameters despite the fact that actual lithium extraction operations display variable conditions. The composition of industrial brine changes because of seasonal effects and evaporation rates and different feed-water sources which impacts both ion transport behavior and electrodialysis performance. Development of a dynamic model needs to prioritize real-time brine chemistry adjustments that modify lithium and magnesium concentrations. The accuracy of predictions would increase through simulations which consider time-dependent factors and variable TDS levels together with competing ions and temperature effects. The model's practical use for industrial lithium extraction operations will improve through the inclusion of actual brine measurement data. The development of multi-stage electrodialysis systems which respond to brine composition changes is essential for maintaining steady lithium selection and recovery efficiency. The performance of electrodialysis as an industrial brine treatment method would improve through addressing its current limitations.

#### Conclusion

The research shows electrodialysis emerges as an efficient technique to extract lithium (Li<sup>+</sup>) from brines containing high Mg<sup>2+</sup>/Li<sup>+</sup> ratios because it facilitates strong Li<sup>+</sup> selectivity along with Mg<sup>2+</sup> rejection by managing ion transport through cation exchange membranes. The simulation data shows that applying 10-15V voltage with current densities between 20-30 mA/cm<sup>2</sup> creates an ideal trade-off between efficient separation and energy efficiency thus making electrodialysis a practical solution for lithium extraction. The large-scale implementation of lithium extraction requires additional membrane engineering and process optimization because the current recovery stages face escalating energy expenses and membrane fouling and concentration polarization issues. Future technological developments of membrane materials alongside hybrid extraction systems and improved electrodialysis configurations will enhance lithium recovery and decrease operational expenses. The research delivers essential computational findings which will help future studies and industrial applications of sustainable lithium manufacturing.

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