Computational Simulation of Lithium Ion Transport through Polymer Nanocomposite Membranes

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Abstract: Presented here are the macroscopic transport mechanisms of lithium ion in clay-polymer nanocomposites membranes with potential use in lithium rechargeable batteries. Computational simulations of the lithium ion transport across the interface of an anode and a cathode provide information to tailor single ion conductors and, thus to enhance ionic conductivity of the membrane. These transport simulations demonstrate that the lithium concentration profile in the nanocomposite membranes decreases linearly as a function of time and position. This finding is surprising because the membranes are single ion conductor with transferences numbers approaching one. Thus, a deeper understanding is needed of the transport properties in a real system, in order to be able to tailor materials with high conductivity and high transference numbers. It is shown that a battery cell with a thinner clay-polymer membrane can deliver a much higher capacity than that of a thicker membrane while the cell voltage remain almost unchanged and under 4 volts.

Key words: lithium battery, clay-polymer, nanocomposite membrane, electrochemical model, transference number

1. INTRODUCTION

We think of membranes as simple devices to facilitate filtration. In fact, membranes play a role in chemical, biological, and engineering processes such as catalysis, separation, and sensing by control of molecular transport and recognition. Critical factors that influence membrane discrimination properties include composition, pore size (as well as homogeneity), chemical functionalization, and electrical transport properties. The membrane community has an increasing interest in using nanомaterials for the production of novel membranes because of the unique selectivity that can be achieved. Clay-polymer nanocomposites show particular promise because of their ease of manufacture (large sheets), their rigidity (self-supporting), and their excellent mechanical properties. However, the process of lithium ion transport through the clay-polymer nanocomposite and the mechanisms of pore size selection are poorly understood at the ionic and molecular level. In addition, manufacturing of clay-polymer nanocomposite membranes with desirable properties has proved challenging.

The objective of this work is to understand and predict the transport mechanisms of the lithium ion in clay-polymer membranes with potential use in lithium rechargeable batteries. Computer simulations of the lithium ion across the interface anode-electrolyte or cathode-electrolyte will provide information to tailor single-ion conductors, and thus enhance the ionic conductivity.

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Lithium ion secondary batteries are the best portable energy storage device available on the consumer electronics market. Improved safety over conventional, fully liquid electrolytes provides a compelling rationale for use of polymer electrolytes in rechargeable lithium batteries, but these polymers often show insufficient conductivity or poor mechanical properties [1]. Still, the ease of film fabrication, ability to withstand electrode volume changes, and low temperature operation of a well-designed polymer-based system provide distinct advantages over many ceramic single-ion conductors. Further research into polymeric or composite single-ion conductors is, therefore, well justified. Sandf et al [2] and Appetecci et al [3] have discussed how composite properties impact battery performance, that is, nanocomposites membranes offer high homogeneity, excellent mechanical properties, and good ionic conductivity when the battery is operated at medium to high temperatures. It is also well established in the literature that inorganic fillers play an important role in the conductivity of these materials, as the interfacial resistance is reduced and the ion mobility enhanced [4, 5]. Of particular interest are the recently formulated clay-polymer membranes [6]. Some modeling work literature is available [7-12] for solid polymer models. In these models, the solid polymer electrolyte contains lithium salts and the transference number is often a fitted equation in function of the lithium salt concentration [10, 12], ion pairing and ion association interactions are important in the electrolyte [7], dilution solution theory describes the transport of the ions in the electrolyte phase [7,9] while the lithium clay-polymer membrane does not contain these salts, except for the lithium present in the gallery and the clay framework and the transference number is independent of the concentration. A large body of modeling work describing secondary lithium batteries has been reviewed and published elsewhere [11]. Our work is an attempt to extend the one-dimensional polymer electrolyte cell model developed by Doyle et al [12] which has shown good agreement with experimental data [13-14], to solid polymer membranes without the present of lithium salts.

In the present paper, the electrochemical transport phenomena of the clay-polymer membranes were developed. The lithium concentration in the membrane was determined at diverse positions by a set of electrochemical parameters found experimentally for the membrane or in the literature for the battery model. In addition, in order to study the performance of the nanocomposite membrane a commonly electrochemical model that represents battery discharge in a single cell battery was modified and used. Our interest using a published electrochemical model that is slightly modified to include polymer nanocomposite membranes properties such as diffusivity, transference number and membrane thickness is to obtain membrane concentration profile and voltage distribution that never have been published for polymer nanocomposite membranes. This model considers the concentration profile, surface overpotential, concentration overpotential, voltage, and the current distribution along the battery cell. Results obtained with this macroscopic model are promising (low cell voltage, low voltage increase when increase of membrane thickness) but there are still many unanswered questions at the molecular level of the mechanism of conduction in these clay-polymer membranes. We are proposing to use molecular dynamic simulation to study the effect of the transference number, membrane thickness, membrane composition, and diffusivity in the lithium ion transport through the clay-polymer membrane.

2. EXPERIMENTAL METHOD

2.1. Synthesis

The clay-polymer membranes used in this work were synthesized as follows. One of the membranes studied was prepared from synthetic lithium Hectorite (SLH). Preparation of the SLH clay via hydrothermal crystallization at 100 °C of silica sol, magnesium hydroxide, and lithium fluoride can be found in detail in Carrado et al. [15]. Colloidal suspensions of 1 g SLH/100 ml de-ionized water were stirred for one-half hour. The desired amount of polyethylene oxide (PEO) (100 000 average molecular weight, from Aldrich) was then added, and the mixture stirred for 24 hours. Mixtures contained 0.6, 0.8, 1.0, and 1.2 g of PEO/g of clay. Films were prepared by puddle-casting the slurries onto Teflon-coated glass plates and air-drying. Further drying was carried out at 120 °C under an inert atmosphere for at least 48 hours. The typical thickness of the films was found to be about 40 µm.

2.2. Electrochemical Model

Here we develop a simplified one-dimensional model for the transport of lithium ions in the clay-polymer membrane. Figure 1 shows the idealized structure of the nanocomposite membrane, which consists of intercalated PEO in the SLH. A schematic representation of a typical Li-ion battery cell is shown in Figure 2. The battery cell consists of three regions: the negative electrode, the clay-polymer membrane, and the porous composite positive electrode. The equations

![Figure 1. Idealized clay-polymer membrane structure of intercalated PEO in the synthetic lithium Hectorite (SLH). Circle dots are represented by the lithium ions, and the PEO chain is shown between the Li ions. (Reproduced with permission of the American Chemical Society Publications).](image-url)
describing the transport of the lithium ion through the porous composite cathode are shown in Appendix A. To simplify the model, we have made the following assumptions: (1) lithium ions are the only ions transported through the membrane; (2) the electroneutrality of the active lithium ions is maintained by coordination of one to six oxygen’s in the PEO chain present in the membrane [16]; (3) the total lithium concentration in the membrane, \( C_0 \), is a known constant parameter; (4) concentration solution theory [17] describes the transport of \( \text{Li}^+ \) ions through the membrane; (5) the diffusion coefficient and the transference number of the \( \text{Li}^+ \) are concentration independent; and (6) only cations are electroactive at the electrolyte-electrode interfaces.

At the Li electrode (\( x = 0 \)), the flux of lithium ions is equal to the dissolution rate of Li, which yields the boundary condition

\[
-D \frac{\partial C}{\partial x} |_{x=0} = \frac{i_{\text{appl}}}{F}.
\]  

(3)

The variation in potential in the membrane is calculated from [18],

\[
\nabla \Theta_2 = -\frac{i_x}{\kappa} - \frac{RT(1 + t_+)}{Z_s \nu_+ F},
\]

(4)

where \( \nabla \Theta_2 \) and \( \kappa \) are the potential and the lithium conductivity in the clay-polymer membrane, respectively. The flux and the concentration of the lithium ion and the potential in the membrane are taken to be continuous from \( x = 0 \) to \( x = L_M \).

### 2.3. Numerical Procedure

The input parameters used in the numerical procedure are listed in Table I. Specific membrane properties such as diffusion coefficient, transference number and membrane thickness are listed in Tables I and II. These membrane properties are used in the simulation to predict the lithium ion transport through the membrane and the impact in battery performance. For the discretization of the model, we used a three-point central difference for both first and second

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_0 )</td>
<td>1,500 mole/m³</td>
</tr>
<tr>
<td>( C_{\text{max}} )</td>
<td>3,600 mole/m³ [10]</td>
</tr>
<tr>
<td>( C_T )</td>
<td>23,700 mole/m³ [10]</td>
</tr>
<tr>
<td>( D_s )</td>
<td>1500 mole/m³ [10]</td>
</tr>
<tr>
<td>( D )</td>
<td>( 1 \times 10^{-11} ) (memb) [22]; ( 8.05 \times 10^{-14} ) (electrolyte) m²/s [10]</td>
</tr>
<tr>
<td>( k )</td>
<td>( 5.9 \times 10^{-3} ) (memb); ( 5.4 \times 10^{-3} ) ohm cm⁻¹ (electrolyte) [10]</td>
</tr>
<tr>
<td>( L_c )</td>
<td>50 μm</td>
</tr>
<tr>
<td>( L_M )</td>
<td>50 μm</td>
</tr>
<tr>
<td>( R_s )</td>
<td>2 μm [10]</td>
</tr>
<tr>
<td>( \alpha_\infty )</td>
<td>0.42 (membrane) [4]</td>
</tr>
<tr>
<td>( \alpha_\text{Li} )</td>
<td>0.42 (electrolyte) [10]</td>
</tr>
<tr>
<td>( \alpha_0 )</td>
<td>0.5 [19]</td>
</tr>
<tr>
<td>( \alpha_c )</td>
<td>0.5 [19]</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>3.8 S/m [21]</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>3.12 x ( 10^2 ) 1/m [10]</td>
</tr>
</tbody>
</table>
derivatives of the partial differential equations and the Crank-Nicholson approximation to obtain accuracy on the order of $\Delta x^2 + \Delta t^2$. Newton-Raphson iteration methods were used to solve the nonlinear equations.

3. RESULTS AND DISCUSSION

Extensive structural and electrochemical characterization have been performed in these membranes and the results have been published elsewhere [2, 5]. In summary, the membranes exhibit excellent conductivity when heated to 60 °C. Small X-ray angle scattering showed that the crystalline regions of the polymer became amorphous at that temperature and the process is irreversible, that is, the polymer relaxes in the clay galleries and does not recover its crystalline nature.

The cationic transference number, $t_+\$, has been found to be a critical property for batteries based on solid polymer electrolytes (SPE) [23]. However, $t_+$ for SPE has proven difficult to measure correctly, and few characterization methods are available. For a similar SPE, significant variations in transport properties can be found as a result of the different methods used [23]. According to studies in Doyle et al [19] and Bouridah et al [24], the transference number is concentration dependent. Experimental results show that the transference number of the clay-polymer membrane is not affected by the salt concentration dissolved in the lattice of the polymer electrolyte [4]. Also, little effect is observed in the transference number for the PEO/SLH ratio used in the membrane preparation. Table II shows that the highest transference number, 0.95, was obtained for a PEO/SLH ratio of 0.8. The transference number of the clay-polymer membrane was over 0.90 as is expected for a single-ion conductor. For the temperature range under study, 25 °C to 150 °C, the transference number remained almost constant.

The biggest increase in the transference number was observed when the temperature increased from 25 °C to 60 °C. At temperatures values beyond 60 °C, this value remained unchanged. The diffusivity of the lithium ion in the polymer nanocomposite membrane has not been measured experimentally. In some cases, a lithium diffusivity value of $1x10^{-11}$ m$^2$/sec [22] was chosen for the simulations.

3.1. Lithium transference number effect

Table II shows the experimental transference numbers obtained for several membrane compositions. The values were calculated following the procedures outlined by Dees et al [25]. It is clearly seen from this table that these nanocomposites membranes behave as single ion conductors, with transference numbers approaching one as the temperature increases and the amorphous regions in the nanocomposite become amorphous.

Several simulations were run at different transference number values while maintaining the current density, temperature, and diffusivity constant. Figure 3 shows the effect of the transference number on the Li$^+$ ion concentration in the clay-polymer membrane for a current density of 0.1 mA/cm$^2$, a temperature of 60 °C and a lithium diffusivity value of $1x10^{-11}$ m$^2$/sec. Letters denote simulation run for (a) $t_{Li^+} = 0.98$, (b) $t_{Li^+} = 0.95$, (c) $t_{Li^+} = 0.90$, (d) $t_{Li^+} = 0.80$, (e) $t_{Li^+} = 0.70$ and (f) $t_{Li^+} = 0.4$.

Table II. Transference numbers obtained for different PEO/SLH mass ratio as a function of temperature.

<table>
<thead>
<tr>
<th>Composition PEO/SLH</th>
<th>Temperature °C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RT</td>
</tr>
<tr>
<td>0.6:1</td>
<td>0.68</td>
</tr>
<tr>
<td>0.8:1</td>
<td>0.80</td>
</tr>
<tr>
<td>1.0:1</td>
<td>0.87</td>
</tr>
<tr>
<td>1.2:1</td>
<td>0.87</td>
</tr>
</tbody>
</table>

3.2. Lithium diffusivity value effect

Transport properties for SPE membranes containing PEO generally show large variations with salt concentration [26-28]. The salt diffusivity may change almost an order of magnitude when the salt concentration doubles [28]. The effect of the Li$^+$ diffusivity value in the clay-polymer membrane is an important parameter to study. The actual lithium diffusivity value in the clay-polymer membrane as a function of the PEO, clay ratio, and temperature is unknown.

Figure 4 shows the profiles of the Li$^+$ ion concentration for a PEO membrane for a current density of 0.1 mA/cm$^2$, a temperature of 60 °C and a lithium diffusivity value of $1x10^{-11}$ m$^2$/sec. The simulations show that, for these conditions, the Li$^+$ ion concentration decreases slightly with the transference number. Ideally, a membrane of transference number equal to 1 should have a constant concentration. For the lowest value, $t_+ = 0.4$, which is a typical transference number for a SPE membrane, the Li$^+$ concentration is reduced by 2% of its initial value. Future simulations should include the effect of the transference number on the performance of the cell battery.
temperature remained constant. We note that for these diffusivity values, the Li⁺ concentration along the clay-polymer remains almost constant with membrane position. When the transference number is decreased to a value of 0.4 while keeping all other parameters constant, it is observed that the concentration profile along the clay polymer membrane varies less than 2% its original lithium concentration for diffusivity values larger than 1x10⁻¹² m²/sec. For the lowest lithium diffusivity, 1x10⁻¹² m²/sec, this concentration change is in the range of 10% (figure not shown).

Figure 4. Predicted concentration profiles of Li⁺ ions in clay-polymer membrane at different membrane Li⁺ diffusivity values. I = 0.1 mA/cm², t⁺ = 0.95 and T = 60 °C. Letters denote simulation run for (a) D Li⁺ = 1.0x10⁻¹⁰ m²/sec, (b) D Li⁺ = 1.5x10⁻¹¹ m²/sec, (c) D Li⁺ = 1.0x10⁻¹¹ m²/sec, (d) D Li⁺ = 1.5x10⁻¹² m²/sec and (e) D Li⁺ = 1.0x10⁻¹² m²/sec.

Figure 5 shows the effect of a low, 0.4 and a high transference number, 0.95 for the lowest membrane diffusivity value, 1x10⁻¹² m²/sec. A 10% decrease of the lithium concentration along the membrane thickness is observed for values of t Li⁺ = 0.4 contrary to a 2% decrease when the transference number is 0.95. From the results shown in Figures 4 and 5, it can be deduced that the membrane concentration is affected by both, diffusivity and transference number.

3.3. Concentration profiles of the lithium ion as a function of time and position in a battery cell

Lithium concentration profiles as a function of the time and position are shown in Figure 6 for three regions: anode, clay-polymer membrane, and cathode of a cell battery. For a given current density (1 mA/cm²), temperature (60 °C), and membrane diffusivity (1x10⁻¹¹ m²/sec), these profiles show that in the clay-polymer membrane region the concentration decreases linearly from x/L = 0 to x/L = 0.5. In the porous cathode region, the lithium concentration decreases near the current collector (x/L = 1) but not along the entire electrode (from x/L = 0.5 to x/L = 1). Profiles at three time intervals — 600, 6300, and 12600 sec — show the described trends; indeed, lithium concentration profiles at t = 12600 sec show that the electrolyte phase of the porous cathode becomes almost depleted. These simulations demonstrate that the lithium concentration in the nanocomposite membrane decreases linearly in the membrane regions as a function of time and position. Because the membranes are single-ion conductors with transference numbers approaching one and the membrane diffusivity chosen to run the simulation is 1x10⁻¹¹ m²/sec, this finding was unexpected. This concentration polarization profile is typical of a lithium salt polymer not of the clay-polymer membrane as found in the simulations run and described previously at different diffusivities and transference numbers. Clearly, a deeper understanding of the membrane properties in a real system is needed in order to be able to tailor materials with high conductivity and high transference numbers.

3.4. Effect of the clay-polymer membrane thickness on state of discharge (L_M = 50 µm and 100 µm)

It is expected that the interfacial cell resistance increases as the thickness of the membranes increases. This has a direct
effect on the overall cell performance and thus, it is desirable to work with thin films in practical cells. Our results indicate that the deliverable capacity of the cell battery assembled with clay-polymer membrane decreases from 100% to 80% with an increase in the membrane thickness from 50 µm to 100 µm (see Figure 7). The cell voltage, however, remains almost unchanged, in the range of 4.3 to 3.9 volts. The voltage profile in this case is different than that obtained using liquid electrolytes. When using liquid electrolytes, there is an excess of ions whereas in the polymer case, there is a well-defined depletion zone that varies as the thickness of the membranes changes.

4. CONCLUSIONS
The mathematical model for porous electrodes developed by Doyle et al. [14] and Song et al. [6] has been reformulated for galvanostatic discharge and has been extended to include the effect of clay-polymer nanocomposite membranes. Transport simulations demonstrate that the lithium concentration profile in the nanocomposite membranes decreases linearly as a function of time and position. This finding was not anticipated because the membranes are single-ion conductors, with transferences numbers approaching one. Further study is needed of the transport properties in a real system, in order to be able to tailor materials with high conductivity and high transference numbers. It has been shown that a battery cell with a thin clay-polymer membrane can deliver a much higher capacity than that of a thicker membrane while the cell voltage remains almost unchanged. In order to predict realistically the performance of the battery cell as a function of design parameters, clay-polymer membrane properties such as diffusivity as function of the PEO/SLH ratio has to be determined accurately.

5. ACKNOWLEDGMENTS
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REFERENCES
APPENDIX A

Cathode composite model. This model, based on assumptions 3, 4, 5, and 6, follows closely that of Doyle et al [12], [19] and Song et al [10].

The material balance for the lithium ion in the composite cathode is

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} + \frac{a j_s (1 - t_1)}{v_r}. \]  

(A-1)

The boundary conditions are

\[ \text{At } x = L_M \quad N_+|_{L_M} = N_+|_{L_M}, \]  

\[ x = L_M + L_C \quad N_+ = 0. \]  

(A-2)

where \( \varepsilon \) is the volume fraction of polymer electrolyte in the cathode; \( a \) is the specific area of the interface between the polymer electrolyte and the solid particles in the composite cathode; \( t_1 \) is the lithium transference number in the electrolyte; \( L_M \) and \( L_C \) are the thickness of the clay-polymer membrane and the composite cathode, respectively; and \( j_s \) is the solid particle surface flux of lithium ions and is related to the divergence of the current flow in the electrolyte phase,

\[ a j_s = - \frac{S_s}{nF} \nabla j_2. \]  

(A-3)

The discharge process consists of the Li\(^+\) insertion in the LiMn\(_2\)O\(_4\), resulting in a two-phase electrode: electrolyte phase and matrix phase [10],

\[ \text{xLi} + \text{LiMn}_2\text{O}_4 \leftrightarrow \text{Li}_{1+x}\text{Mn}_2\text{O}_4. \]  

(A-4)

This leads to a kinetic expression that follows the Butler-Volmer equation

\[ \nabla j_1 = i_0 \left[ \exp \left( \frac{\alpha_F}{RT} \eta \right) - \exp \left( \frac{\alpha_d}{RT} \eta \right) \right] \]  

\[ \eta = aFk \left( C_{\text{max}} - C_0 \right)^n \left( C_I - C_0 \right)^p C_0^q \]  

where \( k \) is the reaction rate constant; \( C_{\text{max}} \) and \( C_I \) are the maximum concentration in the electrolyte and matrix phases, respectively; \( \alpha_F \) and \( \alpha_d \) are the transfer coefficients of anodic and cathodic reactions; and \( \eta \) is the overpotential.

The overpotential of the cathode is obtained from

\[ \nabla \eta = \frac{i_1}{\sigma} + \nabla \Phi_2, \quad I = i_1 + i_2; \quad \text{B.C. } \nabla \eta = -\frac{I}{\sigma} \text{ at } x = L_M + L_C \]  

(A-6)

where \( i_1 \) and \( i_2 \) are the current flow in the matrix and the electrolyte phases, respectively.

If one assumes that the matrix phase is present in spherical particles, the Li\(^+\) insertion process in the matrix phase of the composite cathode can be described by Fick’s diffusion law:

\[ \frac{\partial C_\text{s}}{\partial t} = D_\text{s} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C_\text{s}}{\partial r} \right) \right) \]  

I.C. \( C_\text{s} = C_{\text{i}}^0 \).  

(A-7)

At the center of the spherical particles, \( r = 0 \), the concentration gradient for the inserted Li\(^+\) ions is zero as a result of symmetry:

\[ r = 0 \quad \frac{\partial C_\text{s}}{\partial r} = 0. \]  

(A-8)

At the surface of the solid particles, \( r = R_s \), the flux of the inserted Li\(^+\) into the matrix phase is equal to the electrochemical reaction rate at the surface:

\[ r = R_s \quad j_\text{s} = -D_\text{s} \frac{\partial C_\text{s}}{\partial r}. \]  

(A-9)

The state of discharge (SOD) is related to the intercalation material and calculated by the following equation:

\[ \text{SOD} = \frac{C_\text{i}}{C_{\text{i}}^0} + \frac{It}{L(1 - \varepsilon)C_{\text{i}}^0 F} \]
NOMENCLATURE

- \( a \) specific area of interface between the polymer electrolyte and the solid particles in the composite cathode (1/m)
- \( C \) lithium ions concentration in clay-polymer membrane (mol/m³)
- \( C_0 \) initial concentration of lithium ions (mole/m³)
- \( C_{\text{max}} \) maximum concentration in the electrolyte phase (mole/m³)
- \( C_T \) maximum concentration in the matrix phase (mole/m³)
- \( C_s \) concentration of lithium ions in the matrix phase (mole/m³)
- \( C^0_s \) initial concentration of lithium ions in the matrix phase (mole/m³)
- \( C^* \) saturation concentration of lithium ions in the matrix phase (mole/m³)
- \( D \) diffusion coefficient in a membrane and electrolyte (m²/s)
- \( D_s \) diffusion coefficient in matrix phase (m²/s)
- \( D_F \) Faraday’s constant (96 487 C/mol)
- \( I \) Total current applied also \( i_{\text{app}} \) (mA/cm²)
- \( i_2 \) current density in a clay-polymer membrane and electrolyte phase (mA/cm²)
- \( i_1 \) current density in matrix phase (mA/cm²)
- \( i_0 \) exchange current density at an interface (A/m²) k rate constant (m/s)
- \( j_n \) solid particle surface flux of lithium ions (mol/s m)
- \( L \) length of the cell (µm)
- \( L_e \) length of composite electrode (µm)
- \( L_m \) length of clay-polymer membrane (µm)
- \( N_s \) flux of lithium ions (mol/(m² s))
- \( R \) universal gas constant (8.314 J /mol K)
- \( R_s \) radius of the solid particle (cm²)
- \( r \) radial coordinate (m)
- \( s_i \) stoichiometric coefficient of species i in electrode reaction
- \( t \) time (s)
- \( t_+ \) transference number of Li⁺ ions in clay-polymer membrane and electrolyte
- \( v_+ \) number of cations into which a mole of electrolyte dissociates
- \( x \) coordinate along the cell length (µm)
- \( Z_+ \) lithium charge
- \( \alpha_a \) anodic transfer coefficient
- \( \alpha_c \) cathodic transfer coefficient
- \( \varepsilon \) volume fraction of a phase
- \( \eta \) surface overpotential (V)
- \( \kappa \) conductivity of the electrolyte and clay-polymer membrane (S/cm)
- \( \sigma \) conductivity of the matrix phase (S/cm)
- \( \Phi_1 \) potential in the matrix phase (V)
- \( \Phi_2 \) potential in the clay-polymer membrane and the electrolyte (V)