A Study on the Effect of Porosity and Particles Size Distribution on Li-Ion Battery Performance

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A pseudo two-dimensional model (P2D) is presented that describes the effect of the structural properties of the positive electrode on Li-ion cell performance during discharge. The validation of the mono-modal model was done by using Doyle’s experiment and results (C.M. Doyle, University of California, Berkeley (1995)). A large increase or decrease in the porosity beyond a specific value led to a sharp change in the cell voltage curve and lower cell capacities. The maximum specific energy was obtained in the porosity range of 0.55, while the specific power still had a high value. Furthermore, different particle size distribution models, including mono-modal, bi-modal and 3-particle models, were compared to each other. The mono-modal model was the ideal state with the lowest total polarization. The bi-modal and 3-particle models approached this ideal state when the volume fraction of the smallest particles in their structures increased. This structural arrangement in these models led to more uniform local current density distribution profiles resulting in a greater decrease in cell polarization. Different discharge current densities were applied to different particle size distribution models, and the results showed that the particle size distribution has a greater effect at higher discharge current densities.

Lithium-ion batteries play a significant role in the automotive industry, large-scale utility storage and other advanced technologies due to their beneficial features such as higher energy and power densities along with cycle durability. In addition, the lower environmental impact and improved safety of these new products have clearly demonstrated their advantages as alternatives to fossil fuels.1,2

Since understanding structural properties of batteries is of considerable significance to battery designers in order to improve battery systems, many models have appeared in the literature over the years.3,4

A reaction-zone model based on fast electrode kinetics and neglecting the concentration gradients was first introduced by Newman5 to optimize the electrode thickness and porosity. Ramadesigan et al.6 used a single-electrode model to find the optimal porosity by neglecting the solid-phase intercalation mechanism and considering only the ohmic limitation. The optimization of design parameters, including the thickness and porosity of both electrodes, was done by De et al.7 to maximize the specific energy delivered from the battery; they used a valid reformulated model to facilitate multi-parameter optimization in which the micro structural effects were neglected. Dai and Srinivasan8 described a model based on graded electrode porosity to expand the energy density of the battery.

Until recently, most lithium-ion battery models used a mono-modal particle size distribution for an intercalation electrode, while it is obvious that a real electrode consists of particles with different sizes. Few studies have addressed the effect of particle size on the intercalation electrode performance. Von Sacken et al.9 used an accelerating rate calorimeter to investigate the effect of the specific surface area of the coke used for the negative electrode (LiC6) on the thermal stability. They showed that particle size of the active materials can be beneficial with respect to thermal stability at high temperatures. Tran et al.10 conducted some experiments to study the influence of particle size and discharge rate on the capacity of a lithium-ion graphite electrode. The results showed that the capacity obtained from small graphite particles (6 μm) at a C/2 discharge rate was 80% of that at a C/24 rate (near steady-state conditions). By contrast, the capacity of larger graphite particles (44 μm) at a discharge rate of C/2 was estimated at 25% of the capacity obtained at a C/24 rate. Darling and Newman11 investigated the effect of a bi-modal particle size distribution on galvanostatic cycling using a mathematical model. They indicated that the uniform (mono-modal) particle size distribution should have the lowest conformity to experimental data at a high discharge rate compared to a non-uniform particle size distribution. Meyer et al.12 explained the effect of particle size distribution on the negative electrode and the dependence of local state of charge (SOC) distribution on the distance from the separator. Their results indicated that particles of smaller size, due to their efficient specific surface area, were oxidized faster during the discharge process.

It would appear that a non-uniform particle size distribution in the electrodes is a significant factor to achieve more representative results. Since there are relatively few papers dealing with this important subject in the open literature, it is important to expand the level of knowledge on the effect of different particle size distributions, such as mono-modal, bi-modal and 3-particle size distributions, on the performance of lithium-ion batteries. It should also be stressed that this study is relevant to other battery technologies currently under development, namely high-energy batteries like lithium-air and lithium sulfur.13,14

The presented study follows Doyle’s model15 during the discharge process of a dual Li intercalation cell. The mono-model was extended to the bi-modal and 3-particle size models to study the effect of particle size distributions on cell performance. Firstly, this paper evaluated the effect of different porosities on the specific energy and the specific power of the Li-ion cell. Secondly, the importance of the particle size distributions of the positive electrode on the performance of the cell was studied in detail. Then, the influence of discharge current densities or C-rates on the cell voltage, cell capacity and specific power for different particle size distributions is presented.

Model Development

Modeling a full cell involves the use of complicated coupled partial differential equations. The P2D model is a sophisticated model in which mass and charge transport in the electrolyte and solid phases, as well as the reaction kinetics in the electrolyte-solid interface, are considered. Although this model is more accurate when compared to other models, it is computationally more demanding. Doyle et al.16 developed a P2D model based on the principles of transport phenomena, electrochemistry and thermodynamics. The concentration and potential in the electrolyte, separator and solid phase were found by
solving coupled nonlinear partial differential equations (PDEs), Doyle’s model\textsuperscript{16} was extensively used by other researchers to improve battery systems.\textsuperscript{15,22}

The present work is an extension of Doyle’s model\textsuperscript{15} to bimodal and 3-particle size distribution models. In accordance with his model,\textsuperscript{15} the dual lithium-ion intercalation cell consisted of a negative current collector (Cu), negative porous electrode (Li\textsubscript{x}C\textsubscript{6}), separator, positive porous electrode (Li\textsubscript{y}Mn\textsubscript{2}O\textsubscript{4}) and positive current collector (Al). The plasticized electrolyte was composed of LiPF\textsubscript{6} salt in a liquid mixture of ethylene carbonate and dimethyl carbonate, as well as a copolymer from vinylidene fluoride and hexafluoropropylene. Fig. 1 illustrates a P2D model. All the physical and structural parameters were extracted from Doyle’s model.\textsuperscript{15} A list of these parameters is presented in Table I.

All equations were solved in the x direction except for the Li diffusion equation in solid phase that followed Fick’s law in the r- and where the exchange current density, \( i_0 \), is given by

\[
i_0 = F k \left( c_{1,\text{max}} - c_1 \right)^{n_a} \left( c_i \right)^{n_c} \left( c_2 \right)^{n_a}\]

and where \( k \), \( c_1 \), and \( c_{1,\text{max}} \) and \( c_{1,\text{max}} - c_1 \) are the quasi-equilibrium rate constant; concentration of lithium ions in the electrolyte; maximum concentration of lithium and concentration of the unoccupied sites in the solid phase-negative or positive electrode- respectively.

The surface overpotential was calculated at constant temperature by

\[
\eta_{\text{sur}} = \Phi_1 - \Phi_2 - U \left( c_1 \right)
\]

where \( \Phi_1 \) is the potential in the solid or matrix phase while \( \Phi_2 \) refers to the solution potential. \( U \left( c_1 \right) \) refers to the open circuit potential of the electrode under consideration evaluated at the concentration \( c_1 \) and constant temperature.

Results and Discussion

A summary of the governing equations of the model and the corresponding boundary conditions are presented in Tables II and III.

Numerical Solution

Solving the equations. A time-dependent solver was used to study the cell discharge behavior. The direct solver of MUMPS\textsuperscript{17} was applied to solve the equations. The relative and absolute tolerances were equal to 0.001. The geometry was discretized automatically using a physics-controlled mesh. The maximum solution time was about 10 minutes. The simulated model results are discussed in the next section.

The effect of porosity on cell performance.—Fig. 3 shows the cell voltage curve in terms of cell capacity. The porosity in the positive electrode was considered as a variable while other structural parameters including the thickness of electrodes, separator thickness and negative electrode porosity were kept constant. The end of discharge cell voltage of 3.6 V was chosen for this simulation. With a porosity of 0.65, despite the increased amount of electrolytic solution in the pores of the electrode, a sharp decrease in cell voltage was observed due to the lower amount of active materials, which caused a kinetics limitation in the porous electrode. With a porosity of 0.2, the cell voltage decreased very quickly and the final capacity reached its lowest value. In this situation, despite the fact that the amount of active materials increased, there were not enough Li ions in the solution to reach the reaction zone leading to a mass transfer limitation.

Therefore, it was of significant importance to determine the optimal porosity. To achieve this goal, the cell specific energy was plotted in terms of the specific power of the cell for different porosities in
Table II. Governing equations and boundary conditions for positive and negative electrodes in a pseudo-two dimensional model (x and r).

| Governing equations | Boundary conditions |
|---------------------|---------------------|
| Mass balance in the electrolyte for a binary salt concentrated electrolyte | Positive electrode |
| \( \frac{\partial c}{\partial t} = D_{eff,m} \frac{\partial^2 c}{\partial x^2} + \alpha_m (1 - \rho^2) j_m \) | \(-D_{eff,p} \frac{\partial c}{\partial x}\big|_{x=l_m+b_p} = 0\) |
| Initial condition \( c_1|_{t=0} = c_0 \) | \(-D_{eff,n} \frac{\partial c}{\partial x}\big|_{x=0} = 0\) |
| Hypotheses | Negative electrode |
| Solvent velocity equals to zero | \(-D_{eff, p} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Constant transport properties integrating non-ideality effect | \(-D_{eff, n} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Structural properties-porosity and tortuosity-integrated in \( D_{eff,m} \) | \(-D_{eff, p} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Potential distribution in solution | \(-D_{eff, n} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| \( \nabla \left( -\kappa_{eff,m} \frac{\partial c}{\partial x} + \frac{2 \kappa_{eff,m} RT}{p} (1 - \rho^2) \frac{\ln c}{\Delta x} \right) = \alpha_m F j_m \) | \(-D_{eff, p} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Hypotheses | \(-D_{eff, n} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Structural properties-porosity and tortuosity-integrated in \( \kappa_{eff,m} \) | \(-D_{eff, p} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| Potential distribution in matrix/solid phase | \(-D_{eff, n} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| \( \sigma_{eff,m} \frac{\partial \phi}{\partial x} = \alpha_m F j_m \) | \(\psi_1|_{x=0} = 0\) |
| Hypotheses | \(\sigma_{eff,n}\) \(\frac{\partial \phi}{\partial x}\big|_{x=l_n} = 0\) |
| Structural properties-porosity and tortuosity-integrated in \( \sigma_{eff,m} \) | \(\sigma_{eff,n}\) \(\frac{\partial \phi}{\partial x}\big|_{x=l_n} = 0\) |
| Mass balance-solid-state diffusion only- in the matrix/solid phase in spherical coordinates | \(-D_{eff, p} \frac{\partial c}{\partial x}\big|_{x=l_n} = 0\) |
| \( \frac{\partial c}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D_{m} \frac{\partial c}{\partial r} \right) \) | \(\psi_1|_{x=0} = 0\) |
| Initial condition \( c_1|_{r=0} = c_0 \) | \(\sigma_{eff,n}\) \(\frac{\partial \phi}{\partial x}\big|_{x=l_n} = 0\) |

Table III. Governing equations and boundary conditions for separator.

| Governing equations | Boundary conditions |
|---------------------|---------------------|
| Mass balance in the separator | Positive electrode |
| \( \frac{\partial c}{\partial t} = D_s \frac{\partial^2 c}{\partial r^2} \) | \(-D_{eff,p} \frac{\partial c}{\partial r}\big|_{r=l_s} = 0\) |
| Initial condition \( c_2|_{r=0} = c_0 \) | \(-D_{eff,n} \frac{\partial c}{\partial r}\big|_{r=0} = 0\) |
| Hypotheses | Negative electrode |
| Constant transport properties | \(-D_{eff, p} \frac{\partial c}{\partial r}\big|_{r=l_s} = 0\) |
| No reaction in the separator | \(-D_{eff, n} \frac{\partial c}{\partial r}\big|_{r=l_s} = 0\) |
| Potential distribution in the separator | \(-\kappa_{eff,p} \frac{\partial \phi}{\partial r}\big|_{r=l_s} = 0\) |
| \( \nabla \left( -\kappa_s \frac{\partial c}{\partial r} + \frac{2 \kappa_s RT}{p} (1 - \rho^2) \frac{\ln c}{\Delta r} \right) = \alpha_m F j_m \) | \(-\kappa_{eff, n} \frac{\partial \phi}{\partial r}\big|_{r=l_s} = 0\) |
| \( \psi_1|_{r=0} = 0\) | \(-\kappa_{eff, n} \frac{\partial \phi}{\partial r}\big|_{r=l_s} = 0\) |

Figure 2. Model validation with experimental and simulated data of Doyle.15
Figure 3. Cell voltage as a function of capacity during discharge process for different porosities.

Figure 4. The calculations were done with the constant limit of discharge cell voltage of 3.6 V.

The specific energy and the average specific power of the cell were calculated by

\[
Specific\ Energy = \frac{1}{M} \int_0^{t_f} (I_{\text{app}} \times E_{\text{cell}}) \, dt \quad [5]
\]

\[
Average\ specific\ Power = \frac{Specific\ Energy}{t_f} \quad [6]
\]

where \( M \) and \( I_{\text{app}} \) are the mass per surface area and the current density applied on the positive current collector, respectively, and \( t_f \) is the total discharge time.

According to Fig. 4, there was an increasing trend in the specific energy by increasing the porosity. Then the specific energy reached its maximum value at a porosity of around 0.55, which was followed by a decreasing trend. Therefore, a porosity equal to 0.55 appeared to be the optimal value for such a cell in which both specific energy and specific power have large values.

The effect of different particle size distributions on cell performance.——Three different particle size distribution models were
Table IV. Different particle size distributions.

| Particle size distribution | Radius (μm) | Volume fraction ratio (ε/m) |
|---------------------------|------------|---------------------------|
| Mono-modal                | 8.67       | 1                         |
| Bi-modal                  |            |                           |
| Case 1                    | 8.5        | 0.49                      |
|                            | 8.84       | 0.51                      |
| Case 2                    | 2.34       | 0.135                     |
|                            | 15         | 0.865                     |
| 3-particle model          |            |                           |
| Case 1                    | 4          | 0.265                     |
|                            | 15         | 0.734                     |
|                            | 7          | 0.001                     |
| Case 2                    | 4          | 0.15                      |
|                            | 15         | 0.57                      |
|                            | 7          | 0.28                      |
| Case 3                    | 4          | 0.1                       |
|                            | 15         | 0.5                       |
|                            | 7          | 0.4                       |

selected to study their effect on the cell voltage. In the bi-modal and 3-particle models, the positive electrode consisted of two particles and three particles with different radii, respectively, while the negative electrode was mono-modal. Active material particles were considered as spheres. Furthermore, the volume fraction of the particles was adjusted such that the radius of the mono-modal particle size distribution was the normal average of radii of particles existing in bi-modal or 3-particle size distributions. To create the bi-modal and 3-particle size distribution models, two assumptions were considered according to Darling’s work:

1. The mass of active materials in the bi-modal and 3-particle models was the same as that in a mono-modal model.
2. The specific surface area of the active materials of both bi-modal and 3-particle models was equal to that of the mono-modal model.

The particle radii for the bi-modal and 3-particle models were selected by considering the different ranges of the particle size in their distributions. In addition, the particles with different sizes were considered to be present at all locations in the positive electrode.

According to the above assumptions, the volume fraction of the two particles in a bi-modal model was calculated by

\[ \frac{\varepsilon_{1,b}}{\varepsilon_m} = \frac{r_{1,b}}{r_m} - 1 \]  
[7]

\[ \frac{\varepsilon_{1,b}}{\varepsilon_m} + \frac{\varepsilon_{2,b}}{\varepsilon_m} = 1 \]  
[8]

with \( r_{1,b} < r_m < r_{2,b} \). \( r_{1,b} \) and \( \varepsilon_{1,b} \) are the radius and the volume fraction of the smaller particles in a bi-modal particle size distribution, respectively. \( r_{2,b} \) is the radius of the larger particles in a bi-modal particle size distribution. \( r_m \) and \( \varepsilon_m \) are the radius and the volume fraction of the active material particles in a mono-modal particle size distribution, respectively.

Furthermore, the volume fraction of each particle in a 3-particle model was computed by

\[ \frac{\varepsilon_1}{\varepsilon_m} = \frac{\left( \frac{r_1}{r_m} - 1 \right) - \frac{r_2}{r_m} \left( \frac{r_3}{r_2} - 1 \right)}{\left( \frac{r_2}{r_1} - 1 \right)} \]  
[9]

\[ \frac{\varepsilon_2}{\varepsilon_m} = \frac{\left( \frac{r_1}{r_m} - 1 \right) - \frac{r_3}{r_m} \left( \frac{r_2}{r_3} - 1 \right)}{\left( \frac{r_3}{r_1} - 1 \right)} \]  
[10]

\[ \frac{\varepsilon_1}{\varepsilon_m} + \frac{\varepsilon_2}{\varepsilon_m} + \frac{\varepsilon_3}{\varepsilon_m} = 1 \]  
[11]

By inserting the values of the radii for a specifically selected 3-particle system- \( r_1 = 4 \mu m, r_2 = 15 \mu m \) and \( r_3 = 7 \mu m \) in the above equations (Eqs. 9 and 10), a restricted range of volume fraction was determined such that:

\[ 0 < \frac{\varepsilon_1}{\varepsilon_m} < 0.2655 \]
\[ 0 < \frac{\varepsilon_2}{\varepsilon_m} < 0.361 \]
\[ 0 < \frac{\varepsilon_3}{\varepsilon_m} < 0.6388 \]

Table IV illustrates the ratio of volume fraction of particles in different particle size distribution models to that in mono-modal model.

![Figure 5](image_url) Cell voltage variation with capacity for different particle size distributions.
Fig. 5 shows a comparison of the cell voltage for the mono-modal, bi-modal and 3-particle size distribution models. An ascending trend in cell voltage and capacity was observed by increasing the volume fraction of the smallest particle in both bi-modal and 3-particle size distributions. This difference in cell voltage among model curves resulted from the different distribution of the particles size in the positive electrode structure. According to case 1 of the 3-particle model, the volume fraction of the smallest particle was assumed to have its highest limit ($\varepsilon_1 = 0.265\varepsilon_m$). In this case, the cell voltage reached its maximum value which was less than the cell voltage of the bi-modal model (case 1) and that of the mono-modal structure (as an ideal state). Additionally, the total cell polarization during discharge was higher for case 1 of the 3-particle model compared to that of the bi-modal (case 1) and mono-modal models (Fig. 6).

The total polarization of the cell was calculated by the following equation

$$total\ polarization = E_{OCV,cell} - E_{cell}$$

where $E_{OCV,cell}$ is the open circuit cell voltage.

The total cell polarization increased by decreasing the volume fraction of the smallest particle in both the bi-modal and 3-particle models, as shown in Fig. 6. However, since the initial salt concentration was high enough ($2mol/l$), the concentration polarization caused by diffusion in the solution phase was not of significant impor-

Figure 6. The total cell polarization during discharge time for different particle size distributions.

Figure 7. The electrolyte potential in the direction of thickness of the electrode at the end of discharge ($t = 1800$ s).
By contrast, the ohmic potential drop was the most important contribution to the total polarization for all three models as revealed in Fig. 7. The electrolyte potential along the thickness of the cell for different particle size distribution models is presented in Fig. 7. Despite the fact that the ohmic potential drop was a transport limiting mechanism in all models, the difference in cell total polarization among the different models resulted from the difference in concentration of the different particles in the particle size distribution models. The diffusion polarization in smaller particles is lower compared to that in larger particles because of the lower time constant for diffusion in smaller particles.

Fig. 8 shows the Li concentration of each particle in different particle size distribution models at the surface point close to the positive current collector (point 4, Fig. 1) during discharge. The concentration distributions in each particle arose from the different reaction rates occurring at the surface of the particle. Since the smaller particles have the highest specific surface areas, the Li intercalation reaction was faster. The local current density (A/m²) of the particles of the different particle size distribution models during discharge time is shown in Fig. 9. The results indicate that particle size distribution with different volume fractions affect the local current density distribution. A more uniform local current distribution is observed for case 1 of both bi-modal and 3-particle size distributions, which have a larger volume fraction of the smallest particles compared to that in the other cases. Additionally, the non-uniformity of the local current density increased the total cell polarization as shown in Fig. 6.

The effect of different discharge current densities.—Fig. 10 shows a comparison of the effect of the discharge current densities on the cell voltage and capacity for different particle size distributions. Different current densities were applied in accordance with the following equation

$$I = C \times I_{app}$$

A 1C-rate means a current density that discharges the cell in 1 hour (here it is equal to 17.5 A/m²). At a lower discharge current density (0.1C-rate), there is a good overlap in the mono-modal and all cases of the bi-modal and 3-particle size distributions. However, the cell voltage and cell capacity decreased dramatically at higher current densities (1C-rate and 3C-rate) due to the limitation of Li-ion...
migration toward the reaction zone leading to the increase of the total polarization. There were clear differences among the mono-modal and case 2 of the bi-modal and case 3 of the 3-particle size distribution at higher C-rates. The results indicated that the effect of the particle size distribution was highlighted at higher discharge current densities, and this effect was more pronounced for the 3-particle size distribution even at the highest value of the volume fraction of the smallest particle ($\varepsilon_1 = 0.265\varepsilon_m$). To clarify the effect of the particle size distribution at high discharge current densities, the specific energy curve in terms of the specific power of the cell is shown in Fig. 11. A comparison of the three models at 1C- and 3C-rates for a final discharge cell voltage of 2.8 V is presented. At a higher C-rate, the time required to reach the cutoff voltage decreased and the specific power increased. For both C-rates, the changes in specific energy, in contrast to specific power for the three models, were minor at any specified time due to their same amount of active materials. At a 3C-rate, the differences in specific power for the three models were more distinct than that at a 1C-rate. The highest specific power was obtained with a mono-modal model as an ideal state. The specific power of the two other models was close to the ideal state (mono-modal) by increasing the volume fraction of the smallest particles in their structures.

**Conclusions**

This work focused on studying the effect of porosity and particle size distribution on Li-ion cell performance during the discharge process. The P2D model of Doyle was used to investigate different mass and charge transfer mechanisms in multi-regions of a dual Li intercalation cell. There was good agreement between the cell voltage...
of a mono-modal model simulated by COMSOL Multiphysics 5.2 and Doyle’s results\textsuperscript{15} which showed the validity of our approach.

The mono-modal model was developed further to consider bi-modal and 3-particle models to study the effect of particle size distribution in the positive electrode on the overall cell performance. The results showed that there is an optimal porosity beyond which lower cell capacities are observed due to the kinetics and mass transfer limitations in the porous electrode. A porosity of around 0.55 was found as the optimum value for achieving the maximum specific energy while an acceptable amount of specific power was sacrificed.

To study the effect of particle size distributions, mono-modal and bi-modal and 3-particle models with different volume fractions of small and large particles were considered. The results showed that increasing the volume fraction of the smallest particles in both bi-modal and 3-particle models increased the cell voltage and decreased total polarization. The non-uniformity of local current densities on particle surface was the reason of the difference among the models.

The effect of different discharge current densities or C-rates on the cell performance of different particle size distribution was studied. The effect of the particle size distribution on cell voltage, capacity and specific power was more pronounced at higher C-rates. The results showed that at 3C-rate, the difference in the specific power among the different particle size distribution models was more significant than that at 1C-rate.

Figure 10. A comparison of the effect of the different discharge current densities on cell voltage of (a) mono-modal and bi-modal (b) mono-modal and 3-particle size distribution models.
Overall, the results indicated that the volume fraction of small and large particles in a bi-modal or 3-particle model has a profound effect on battery performance characteristics such as cell capacity, voltage and specific power. In fact, by increasing the portion of the smallest particles in each model, the behavior of the bi-modal and 3-particle models was closer to that of the mono-modal model as an ideal state.

For future work, the purpose of the authors is to develop approaches that will consider the effect of particle size distribution in the simplest way for system and engineering developers. This would involve a link between experimental works dedicated to PSD characterization (microscopy for example) and modeling. In addition, the arrangement of particles with different sizes in the electrodes based on the distance from separator or current collector is another important aspect to consider. It could be the subject for our next study.

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List of Symbols

- $a$: Specific surface area, m²/m³
- $c$: Concentration of Li, mol/m³
- $c_0$: Initial concentration of lithium in the solid phase, mol/m³
- $c_{\text{max}}$: Maximum concentration of lithium in the solid phase, mol/m³
- $D$: Diffusion coefficient, m²/s
- $F$: Faraday’s constant, 96487, C/mol
- $i_0$: Exchange current density, A/m²
Local current density in the porous matrix, $A/m^2$

Applied current density of cell, $A/m^2$

Pore wall flux of lithium-ions, $mol/m^2 s$

Reaction rate constant

Thickness, $m$

Mass per surface area of cell, $kg/m^2$

Radial coordinate, $m$

Universal gas constant, $8.314 \text{ J/mol K}$

Time, $s$

Transference number of species Li$^+$

Absolute temperature, $K$

Open-circuit potential, $V$

Spatial coordinate, $m$

Subscripts

$ef$ Effective value of transport property in porous medium

$n$ Negative electrode

$p$ Positive electrode

$s$ Separator

$1$ Solid phase

$2$ Solution phase

Greek

$\alpha_a, \alpha_c$ Anodic and cathodic transfer coefficients

$\varepsilon$ Volume fraction or porosity of a phase

$\eta$ Overpotential, $V$

$\kappa$ Ionic conductivity of electrolyte, $S/m$

$\sigma$ Electronic conductivity of the solid phase, $S/m$

$\Phi$ Electrical potential, $V$

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