

# ***Modeling & Simulation of Li-ion batteries using Doyle-Fuller-Newman (DFN) Model***

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**Introduction:** Batteries powered by lithium-ion are important in various applications, such as electric cars, portable electronic devices, intelligent grid systems, and renewable energy systems. These batteries are a good option for various applications due to their high energy density, long cycle life, and low self-discharge. Nevertheless, the performance of lithium-ion batteries can be impacted by various factors, such as the electrode material, the composition of the electrolyte, the operating circumstances, and the cycling history. It is essential to have an in-depth understanding of the complicated physical and chemical processes inside a battery to improve the performance of existing battery technologies and develop new ones. The Doyle-Fuller-Newman (DFN) model is a sophisticated mathematical model that can mimic the behavior of lithium-ion batteries and give insights into the underlying physics of how batteries operate.

Batteries are omnipresent. Technologies pertaining to control systems that augment the performance of batteries are of great significance. Electrochemical control systems based on models offer insight into the operational conditions that lead to degradation. The enhanced visibility facilitates an expanded operational range that leads to improved energy and power capacities as well as accelerated charging rates, as stated in reference [1]. The process of state estimation based on electrochemical models presents significant technical difficulties. The system of nonlinear partial differential algebraic equations [2], [3] governs the dynamics. Furthermore, it should be noted that the global observability of local states is not guaranteed, as indicated in reference [4]. Thirdly, it should be noted that the parameters of the model exhibit significant variation depending on factors such as electrode chemistry, electrolyte composition, packaging, and duration. Battery pack cells typically exhibit heterogeneity in terms of their parameters, temperature, and state of charge (SOC). Acquiring a comprehensive comprehension of the mathematical model structure is a driving force behind the development of an observer design.

Electrochemical models are utilized to consider diffusion, intercalation, and electrochemical kinetics. The mathematical structure of these models poses a challenge in designing observers, despite their ability to precisely forecast internal state variables. As a result, the majority of methodologies focus on creating estimators for models with lower orders. The process of model reduction and observer design are closely interconnected, as the utilization of less complex models facilitates the design of estimations but results in a decrease in accuracy. The objective is to obtain a stable estimator that can be proven to be reliable for the most accurate electrochemical battery model achievable.

The fundamental purpose of this project is to use the DFN model to gain a thorough knowledge of the behavior of lithium-ion batteries. The DFN model will be used to assist in the construction of a full-scale model of a lithium-ion battery. Examining the impacts of important factors on the functioning of the battery, such as the electrodes' thickness, the electrolyte's concentration, and the number of times the battery has been cycled. The battery's design is optimized to increase its performance under particular operating circumstances.

A thorough examination of observer estimating error stability, SPM (Single Particle Model) dynamics estimation investigations, and lithium conservation are absent. All of these techniques also depend on a specific method of numerical discretization. In other words, they instantly discretize the partial differential equations (PDEs) before using analysis and estimating synthesis in the finite-dimensional domain.

Prior to discretization, the PDEs are subjected to analysis, and estimating synthesis has the following two benefits:

- 1) If the discretization method is changed, the estimator design need not be re-done; and
- 2) Regardless of the discretization method used at the implementation stage, the physical significance of the equations (and of the phenomena they represent) is retained, providing valuable insights as a byproduct of the design process that is lost in other approaches. Unfortunately, as model complexity rises, it becomes harder to demonstrate estimation error stability. The main problem is that total observability from voltage measurements is lacking.

**Objective:** The primary goal of this report is to use the DFN model to create mechanistic knowledge about the behavior of Li-ion batteries. The DFN model includes the following characteristic equations:

- Transport equation for lithium-ion concentration
- Transport equation for electrolyte concentration
- Transport equation for electrolyte potential
- A Butler-Volmer equation for electrode kinetics
- Equation for the solid-electrolyte interphase (SEI) formation
- Equation for thermal effects

In this project, the focus of the study is on the physics phenomena like diffusion, migration, and deintercalation from anode during discharging, considering the chemical parts of the equation as fixed. All the equations of the DFN model are mentioned in reference 1.

The project's precise goal consists of the following-

1. Building a full equation model using a set of the equation of the DFN model for electrode and electrolyte in 1- dimensional space.
2. Scaling down the PDE equation on Li-ion concentration change due to diffusion in both solid phase and electrolyte phase.
3. After scaling down, some non-dimensional parameters arrive in the equation.
4. Some physical parameters, such as the radius of the particle, the thickness of the anode, the charge rate, etc., varied to see their effect on the non-dimensional parameter and voltage output of the battery.
5. Try to evaluate the estimation of the analytical result with COMSOL result output and report the deviation.

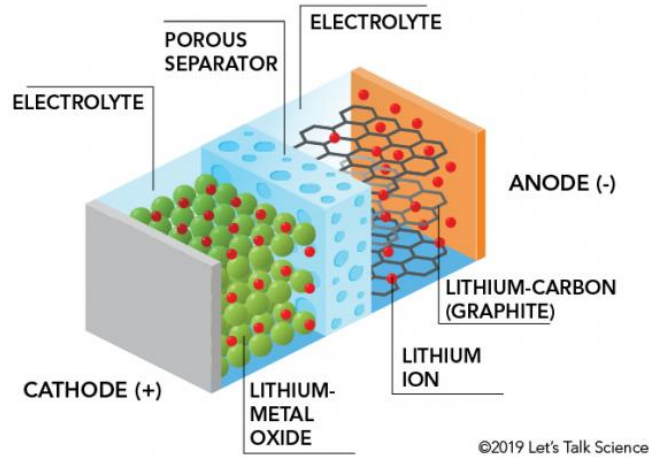
### **Advantages of the DFN Model:**

- Comprehensive description of electrochemical processes
- Accurate prediction of battery performance
- Ability to simulate different battery chemistries and designs
- Insight into the behavior of the battery under different operating conditions
- Potential for optimization of battery design and performance

### **The assumption for the DFN model:**

- The battery is a homogeneous and isotropic material with uniform electrode thickness and properties.
- The electrodes and electrolyte are in a steady-state condition, with no significant variations in temperature, pressure, or composition over time.
- The model assumes that the battery is operating under a constant current or constant voltage regime with no transient or intermittent current flows.
- The battery is free of defects or irregularities, such as cracks, voids, or inclusions, that could impact its performance or behavior.
- Considering the battery as a closed system, with no significant mass transfer or chemical reactions occurring at its boundaries.
- The model assumes that the diffusion coefficient is a dependent function of concentration.
- The total moles of Li-ion in the electrolyte  $n_{\text{Li,e}}$  is conserved. This assumption is considered in the boundary condition of electrolytes 6-9.
- Electrolyte is a concentrated solution.
- Electrodes are porous, and charge in the whole cells is conserved. This is considered a porosity factor in equation 4.
- Electrochemistry part of the DFN equation is not taken into account in this study.

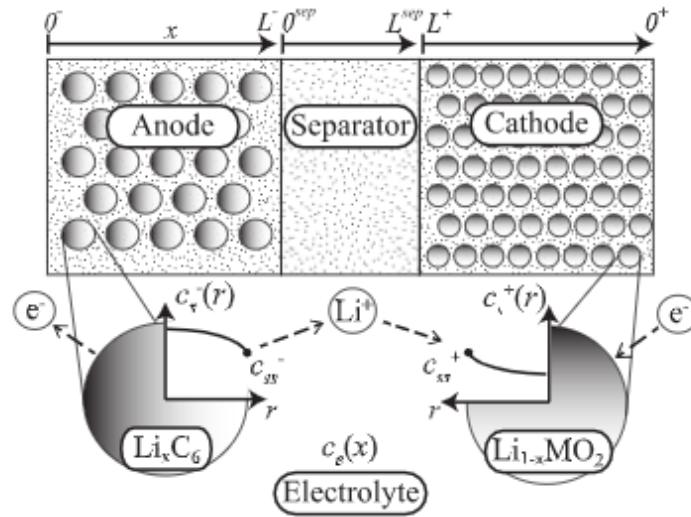
Li-ion batteries consist of an anode, cathode, and separator. Cathode is Li metal oxide, and the anode is lithiated graphite, Solid polymer is considered a separator. Most of the time electrolyte is  $\text{LiPF}_6$ . Along with concentrated electrolyte, and Ethylene carbonate, the solution is added as a solvent to stabilize the electrolyte during operation. Various oxidation and reduction occur in batteries during different phase operations of LiBs. Those kinetics reactions are for charging-discharging intercalation, SEI formation, plating formation, etc. DFN equations are based on concentrated solution theory in a binary salt solution for a porous electrode, where it is mentioned that mass transfer depends on the gradient of chemical potential. The separator in Li batteries consists of electrolytes and solvents.



**Figure1:** Schematic Parts of a lithium-ion battery [5]

### **The equations and Corresponding Boundary Condition:**

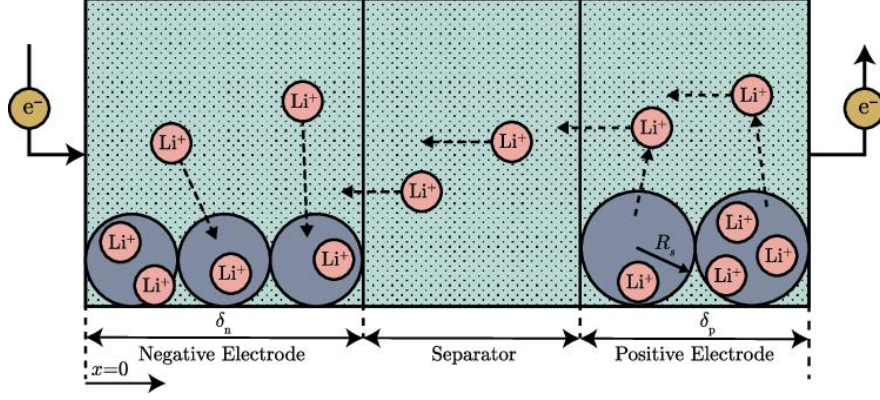
DFN equation contains 21 sets of equations considering different physical and electro-chemical phenomena. [1] The system of equations considered in this project includes the physical phenomena like diffusion of lithium ions in solid particles, diffusion and migration of lithium ions in liquid electrolytes, current distribution, and deintercalation of li-ions during discharge.



**Figure 2:** Schematic of the DFN model. The model considers two phases: the solid and the electrolyte. In the solid, states evolve in the  $x$  and  $r$  dimensions. In the electrolyte, states evolve in the  $x$  dimension only.

The cell is divided into three regions: anode, separator, and cathode [1]

In this study, the physics parameter during discharge is only taken into account. In this report, chemical phenomena and electro-chemical interactions are not taken into account explicitly. Hence, the DFN equations mentioned in related to chemical reactions, such as Butler Volmer kinetics and voltage-current distribution, are not considered in this model.



**Figure 3:** DFN model in Li-cell [2]

Li-ion concentration distribution equation in solid electrode and liquid as per DFN model [1,2]-

Transport equation for Solid state diffusion of lithium ions-

$$\frac{\partial c_s^\pm}{\partial t}(x, r, t) = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_s^\pm r^2 \frac{\partial c_s^\pm}{\partial r}(x, r, t) \right] \quad (1)$$

It is derived from Fick's 2<sup>nd</sup> law of diffusion for spherical particles considering the radial symmetry.

Boundary Condition for Solid State Diffusion as per Equation 1:

$$\frac{\partial c_s^\pm}{\partial r}(x, 0, t) = 0 \quad (2)$$

$$\frac{\partial c_s^\pm}{\partial r}(x, R_s^\pm, t) = -\frac{1}{D_s^\pm} j_n^\pm(x, t) = -\frac{1}{D_s^\pm F a^\pm L^\pm} i_n^\pm(x, t) \quad (3)$$

Transport equation for movement of lithium ions in electrolyte-

$$\epsilon_e^j \frac{\partial c_e^j}{\partial t}(x, t) = \frac{\partial}{\partial x} \left[ D_e(c_e^j) \frac{\partial c_e^j}{\partial x}(x, t) + \frac{(1 - t_c^0) i_e^j(x, t)}{F} \right] \quad (4)$$

Where,  $j \in +, 0, -$ , + for cathode, - for anode, 0 for separator

It is derived from the convective-diffusion equation for total flux in electrolyte due to diffusion, migration and convection. But in this case, no convection occurs. Hence,  $C_j v = 0$

$$J_i = -D_j \nabla C_j - \frac{z_j F}{RT} D_j C_j \nabla \phi + C_j v$$

Boundary Condition for movement of lithium ions in electrolyte as per equation 4:

$$\frac{\partial c_e^-}{\partial x}(0^-, t) = \frac{\partial c_e^+}{\partial x}(0^+, t) = 0 \quad (5)$$

$$D_e^{-,eff}(c_e(L^-)) \frac{\partial c_e^-}{\partial x}(L^-, t) = D_e^{sep,eff}(c_e(0^{sep})) \times \frac{\partial c_e^{sep}}{\partial x}(0^{sep}, t) \quad (6)$$

$$D_e^{sep,eff}(c_e(L^{sep})) \frac{\partial c_e^{sep}}{\partial x}(L^{sep}, t) = D_e^{+,eff}(c_e(0^{se+})) \times \frac{\partial c_e^+}{\partial x}(0^+, t) \quad (7)$$

$$c_e(L^-, t) = c_e(0^{sep}, t) \quad (8)$$

$$c_e(L^{sep}, t) = c_e(0^+, t) \quad (9)$$

Here,

c- Concentration

R= Particle Outer radius

D= Diffusion

D= Diffusion constant

L=Thickness of the electrode

i= current flux into the particle

t= time scale

$\epsilon$ = porosity of electrolyte

x= length scale

$t_c$ = Transference number

r= radius scale

z= no of ions,

R= Universal gas constant

T= temperature

$j_n$ = Lithium flux in anode

Subscript p for cathode and n for anode,

a= surface area

0 for separator, s for solid, e for electrolyte

All other parameter is mentioned in Appendix 2.

Here, this project focuses on the voltage change due to the variation of Li-Ion flux. The parameters involved in the variation of flux are shown below-

- Radius of Anode Particles ( $r_n$ )
- Radius of Cathode Particles ( $r_p$ )
- Diffusion Co-efficient of anode particle ( $D_s$ )
- Thickness of Anode ( $L_n$ )
- Charging/Discharging rate (*C rate*), (Total Charging/Discharging current, = C rate x Total applied current(I) at 1C rate)

**Nondimensionalization and Analysis:** After nondimensionalization all the equations, some critical parameters are found whose effect are the determining factor in the equation.

**Table1: Scaling Parameter**

	Nondimensionalized parameter found from solid state diffusion equation 1-3			Nondimensionalized parameter found from liquid state movement of Li ion equation 4-9
1	Time $\tilde{t} = \frac{t}{t_0} = \frac{t \cdot D_s}{R^2}$		6	Length Scale, $\tilde{x} = \frac{x}{L}$
2	Time scale factor, $t_0 = \frac{R^2}{D_s}$ ,  from equation 1, this time scale also applied to liquid phase li ion movement		7	Diffusion Scale, $\tilde{D}_e = \frac{D_e^{eff}}{D_s}$

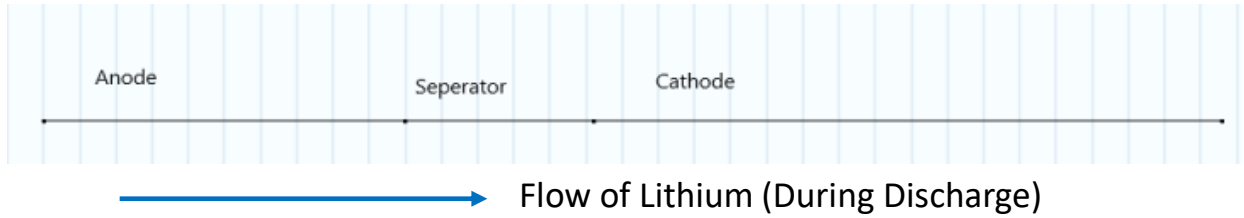
3	Li concentration in porous particle factor, $\tilde{c} = \frac{C_s}{C_{max}}$	8	Liquid phase Li concentration dependence factor, $A = \frac{R^2}{L^2 \cdot \epsilon_e}$ From equation 4
4	Particle radius, $\tilde{r} = \frac{r}{R}$	9	Liquid phase Li concentration factor, $\tilde{c}_e = \frac{c_e^j}{C_0}$
5	Diffusion flux scaling parameter, $M = \frac{C_{max} \cdot D_s \cdot F a L}{R \cdot I}$ , from equation 3	10	Current Scaling, $\tilde{i}_e = \frac{i_e}{I}$
		11	Migration constant in Liquid electrolyte $N = \frac{(1 - t_0) \cdot I \cdot L}{F \cdot D_s \cdot C_0 \cdot a}$ From equation 4

After nondimensionalization, some critical factors are arrived in the equations. All the equations consisting critical parameter mentioned below-

**Table 2:** Equation consisting scaling parameter

$\frac{\partial \tilde{c}_s}{\partial \tilde{t}}(\tilde{x}, \tilde{r}, \tilde{t}) = \frac{1}{\tilde{r}^2} \frac{\partial}{\partial \tilde{r}} [\tilde{r}^2 \frac{\partial \tilde{c}_s}{\partial \tilde{r}}(\tilde{x}, \tilde{r}, \tilde{t})]$ , derived from equation 1	(10)
$M \frac{\partial \tilde{c}_s^+}{\partial \tilde{r}}(\tilde{x}, 1^+, \tilde{t}) = -\tilde{I}_n^\pm$ , derived from equation 3	(11)
$\frac{\partial \tilde{c}_e^j}{\partial \tilde{t}}(\tilde{x}, \tilde{t}) = A \frac{\partial}{\partial \tilde{x}} [\tilde{D}_e \frac{\partial \tilde{c}_e^j}{\partial \tilde{x}}(\tilde{x}, \tilde{t}) + N \tilde{i}_e^j(\tilde{x}, \tilde{t})]$ , derived from equation 4	(12)
Liquid phase Li concentration dependence factor, $A = \frac{R^2}{L^2 \cdot \epsilon_e}$ , derived from equation 5	(13)
Migration constant in Liquid electrolyte, $N = \frac{(1 - t_0) \cdot I \cdot L}{F \cdot D_s \cdot C_0 \cdot a}$ , derived from equation 5	(14)
$\frac{\partial \tilde{c}_s^\pm}{\partial \tilde{r}}(\tilde{x}, 0, \tilde{t}) = 0$ , derived from equation 2	(15)
$\frac{\partial \tilde{c}_e^\pm}{\partial \tilde{x}}(0^-, \tilde{t}) = \frac{\partial \tilde{c}_e^\pm}{\partial \tilde{x}}(0^+, \tilde{t}) = 0$	(16)
$\tilde{D}_e^{-,eff}(\tilde{c}_e(\tilde{L}^-)) \frac{\partial \tilde{c}_e}{\partial \tilde{x}}(\tilde{L}^-, \tilde{t}) = \tilde{D}_e^{sep,eff}(\tilde{c}_e(0^{sep})) \times \frac{\partial \tilde{c}_e^{sep}}{\partial \tilde{x}}(0^{sep}, \tilde{t})$	(17)
$\tilde{D}_e^{sep,eff}(\tilde{c}_e(\tilde{L}^{sep})) \frac{\partial \tilde{c}_e^{sep}}{\partial \tilde{x}}(\tilde{L}^{sep}, \tilde{t}) = \tilde{D}_e^{+,eff}(\tilde{c}_e(\tilde{0}^{sep+})) \times \frac{\partial \tilde{c}_e^+}{\partial \tilde{x}}(\tilde{0}^+, \tilde{t})$	(18)
$\tilde{c}_e(\tilde{L}^-, \tilde{t}) = \tilde{c}_e(\tilde{0}^{sep}, \tilde{t})$	(19)
$\tilde{c}_e(\tilde{L}^{sep}, \tilde{t}) = \tilde{c}_e(\tilde{0}^+, \tilde{t})$	(20)

Due to complexities involved, DFN equations are solved in COMSOL battery solver with a 1D assumption for batteries. The parameter used in the modeling mentioned in the reference.



**Figure 4:** 1-D battery modeling

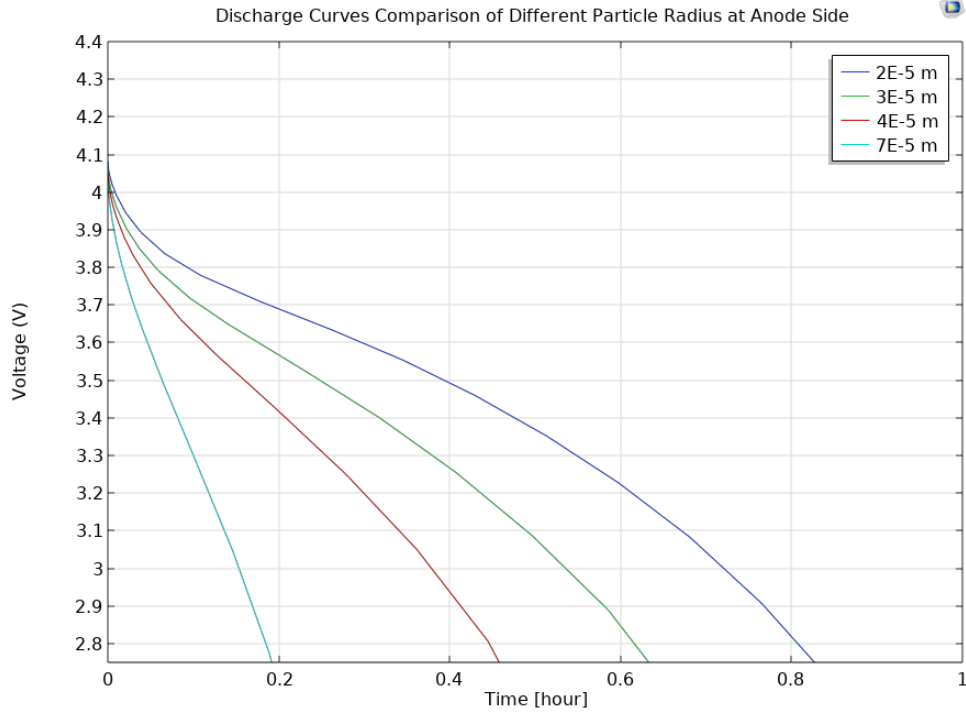
**Table 3:** Range for Dimensionless Parameter

Scaling Parameter	Typical Range value used in this project
$t_0$	$(2 \sim 125.64) * 10^3$
M	$(1.47 \sim 75.4) * 10^{-6}$
N	$(0.447 - 2.36) * 10^6$
A	$(0.024 \sim 0.294) * 10^{-9}$

### **Result and Discussion:**

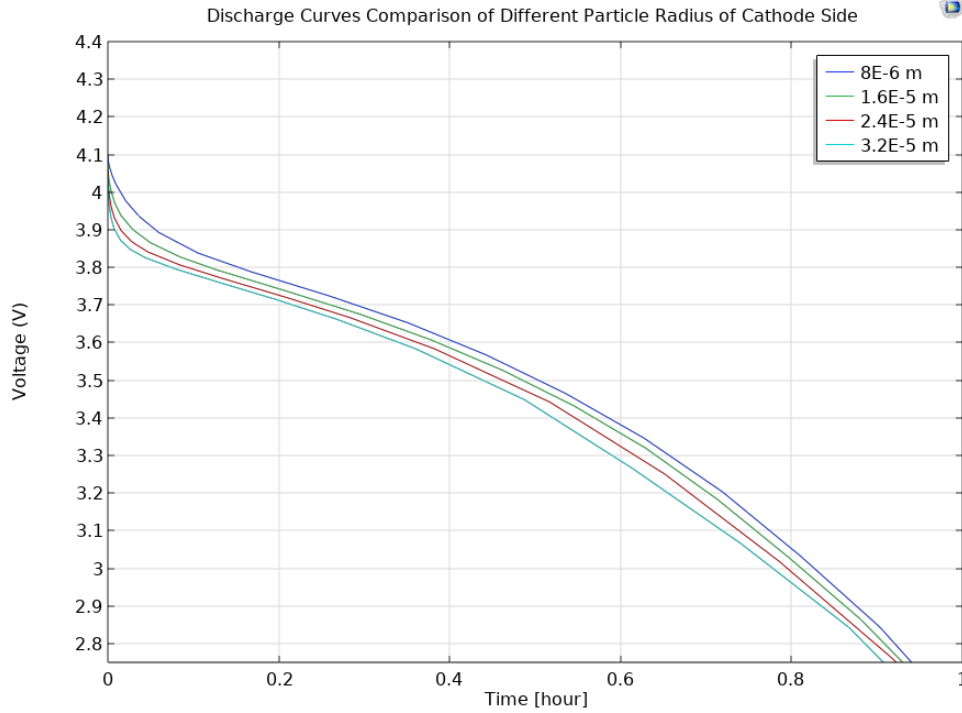
The simulation is done in 1D model for battery simulation module of COMSOL. All the parameter used in COMSOL simulation is describe in appendix 1. The COMSOL simulation is done with a variation in parameter like Anode particle radius( $r_n$ ), Diffusion Constant in Anode Particle ( $D_s$ ), Thickness of Anode ( $L_n$ ), Cathode Particle Radius ( $R_p$ ) and Current Rate (C rate). In figure 5, different particle radius of anode is used to understand the change in voltage. It is found that increase in radius of anode particle directly related to decrease in the diffusion flux scaling parameter M. From equation 10,11, it can be concluded that decrease in M signifies increase in surface concentration of particle within less time which eventually shows as less time required for larger anode particle to 3.0V during discharge.





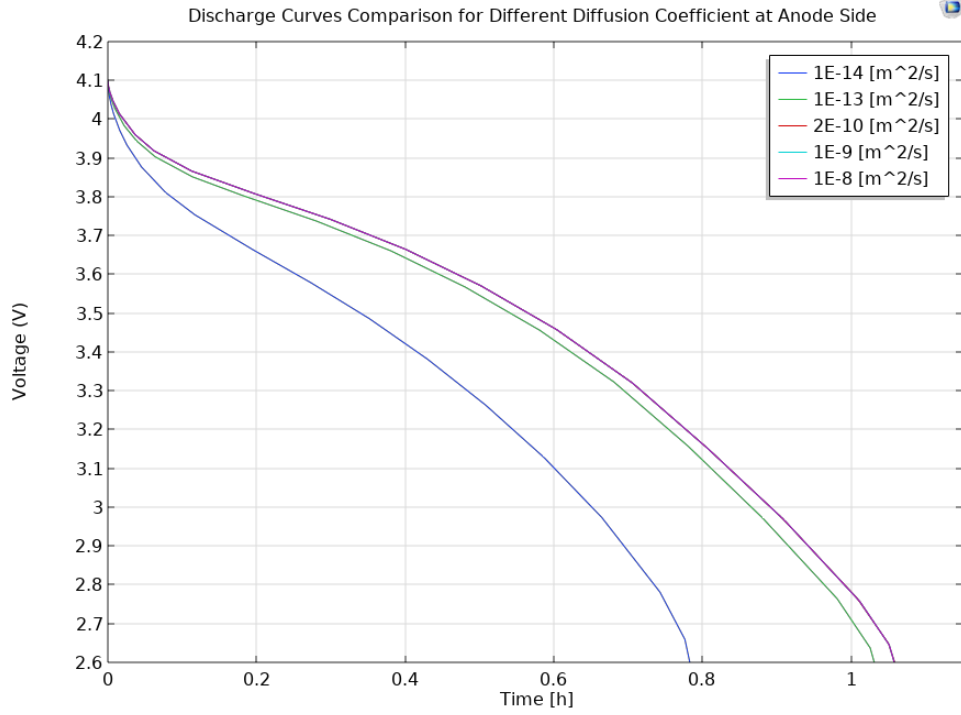
**Figure 5:** Discharge Curves Comparison of Different Particle Radius at Anode side

Similarly, in figure 6, with a variation in parameter like Cathode particle radius( $r_p$ ) keeping all other parameter constant, it is found that increase in radius of cathode particle radius directly related to decrease in the diffusion flux scaling parameter  $M$ . From equation 10,11, it can be concluded that decrease in  $M$  signifies increase in surface concentration of particle within less time which eventually shows as less time required for larger anode particle to 3.0V during discharge. One point needs to be kept in mind, this study done during the discharge phase hence, li-ion particle comes from anode. Hence, source term for Li ion is constant. That's why, the effect on Cathode particle radius( $r_p$ ) is not very significant during discharge.

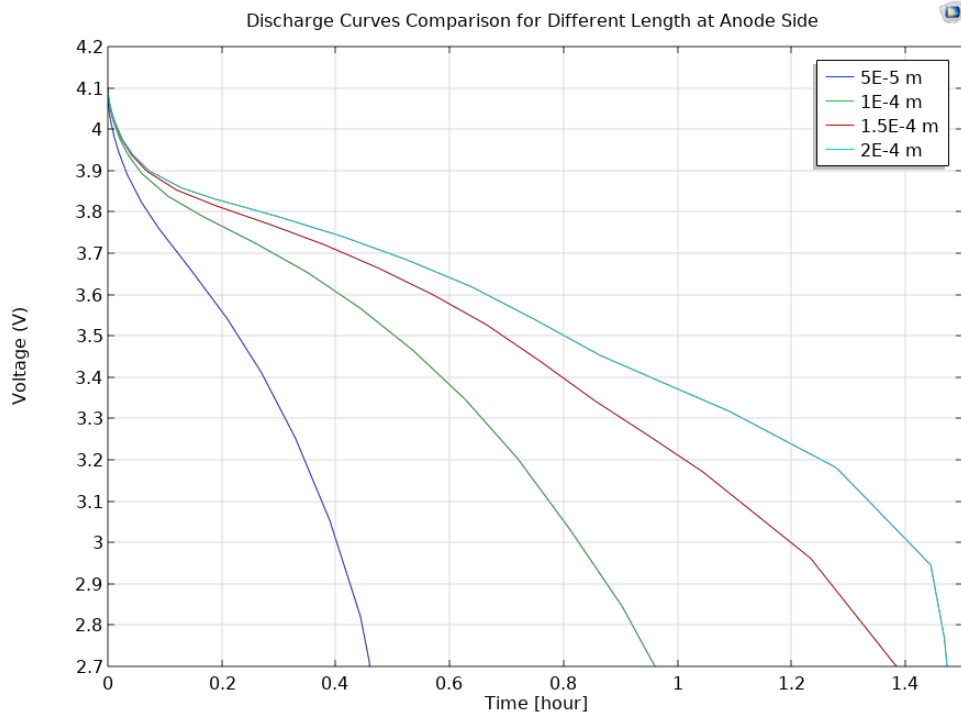


**Figure 6:** Discharge Curves Comparison of Different Particle Radius at Cathode side

In figure 7, it is found that an increase in diffusion coefficient is not significantly affect the lithium flux coming out from the anode particle. Increase in diffusion coefficient is related to decrease in the parameter  $t_0$ . And increase in parameter  $M$ . It signifies, higher the diffusion constant, higher time required to decrease the surface concentration of the particle which is proportionally related to voltage. This understanding is completely in line with the COMSOL result in figure 7. Another finding can be highlighted that decrease in diffusion coefficient beyond certain limit, significantly reduces the time required to reach the cut off voltage.



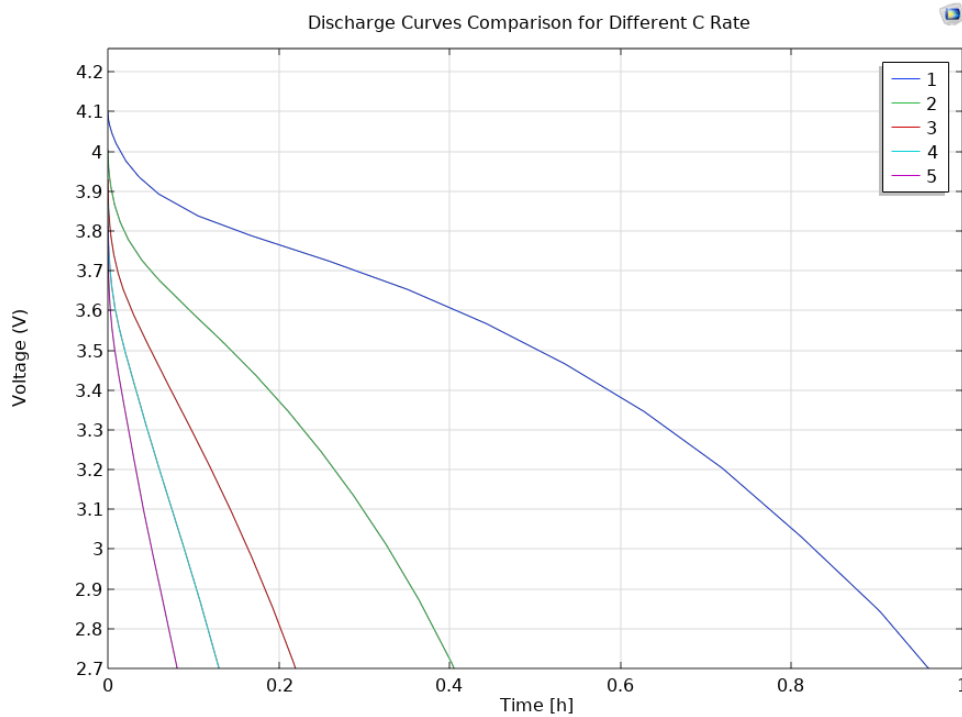
**Figure 7:** Discharge Curves Comparison for different diffusion coefficient at anode side



**Figure 8:** Discharge Curves Comparison for different anode thickness at anode side

In figure 8, anode thickness is varied from  $2\text{e-}4$  m to  $5\text{e-}5$  m. It is found that an increase in anode thickness is related to decrease in the liquid phase Li concentration dependence factor A. From equation 12, it is found that decrease in effect the total li-ion flux to reduced moving inside the

anode region of the cell. As flux reduces, the time to reach cut off voltage increase. The understanding from nondimensionalization on anode thickness variation is totally in line with the COMSOL result.



**Figure 9:** Discharge Curves Comparison for different C rate

In figure 9, Discharge rate is varied from 1C to 5C. It is found that an increase in C rate is related to increase in the current flux which eventually increase the total current flux due to migration which showed an increase in migration constant  $N$  in liquid electrolyte. Increase in total flux signifies, lesser time required to reach 3.0V during discharge. This estimation is totally same as per COMSOL result in figure 9.

**Conclusion:** The objective of this study is to get a full understanding of the behavior of lithium-ion batteries using the DFN model. This project helps us to understand critical parameter affecting most in the behavior study of the Li battery. It also helps us to get brief review like for diffusion and migration phenomena in Li battery is highly dependent on radius of the particle, thickness of the electrode, diffusion constant and applied current flux. The initiative is anticipated to give important insights into the fundamental physics of battery functioning and serve as a platform for future battery research. In this study, no degradation mechanism is not considered. Along with for simplification purposes, initial Li distribution considered to be constant. Due to complexities in numerical solving, current is considered as constant during particular phase. Overall, this study helps us understand different critical dimensionless parameter determining the functionalities of battery.

## **Future Work:**

- Improving the accuracy and efficiency of the DFN model, particularly in simulating complex electrochemical reactions and transport phenomena.
- Using the DFN model to explore new electrode and electrolyte materials, as well as to optimize existing materials for better performance and longer life.
- Developing new battery architectures and designs based on insights gained from the DFN model, such as 3D-printed electrodes and solid-state electrolytes.
- Applying the DFN model to study battery degradation mechanisms, including capacity fading, impedance growth, and dendrite formation, with the goal of developing strategies to mitigate these effects and extend battery life.
- Using the DFN model to optimize battery performance for specific applications, such as electric vehicles, grid storage, and portable electronics.
- Integrating the DFN model with other modeling and simulation tools, such as machine learning algorithms, to enable faster and more accurate battery design and optimization.
- Developing experimental techniques to validate and refine the predictions of the DFN model, and to provide feedback for further model development and improvement.

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6. Rahimian, Saeed Khaleghi, Sean Rayman, and Ralph E. White. "Extension of physics-based single particle model for higher charge–discharge rates." Journal of Power Sources 224 (2013): 180-194.

## **Appendix 1**

Reference parameter used in COMSOL analysis:

Name	Value	Description
brugg	3.3	Bruggeman coefficient
C	1	C-rate factor for the parametric study
cl_0	2000 mol/m <sup>3</sup>	Initial electrolyte salt concentration
cl_ref	2000 mol/m <sup>3</sup>	Reference electrolyte salt concentration
cs_neg_ref	14870 mol/m <sup>3</sup>	Reference concentration negative active electrode material
cs_pos_ref	3900 mol/m <sup>3</sup>	Reference concentration negative active electrode material
cs0_neg	14870 mol/m <sup>3</sup>	Initial concentration negative active electrode material
cs0_pos	3900 mol/m <sup>3</sup>	Initial concentration positive active electrode material
csmax_neg	26390 mol/m <sup>3</sup>	Max solid phase concentration, negative electrode
csmax_pos	22860 mol/m <sup>3</sup>	Max solid phase concentration, positive electrode
Ds_neg	3.9E-14 m <sup>2</sup> /s	Solid phase Li-diffusivity negative electrode
Ds_pos	1E-13 m <sup>2</sup> /s	Solid phase Li-diffusivity positive electrode
eps_l_neg	0.503	Electrolyte phase volume fraction, negative electrode
eps_l_pos	0.63	Electrolyte phase volume fraction, positive electrode
epss_filler_neg	0.026	Conductive filler phase volume fraction, negative
epss_filler_pos	0.073	Conductive filler phase volume fraction, positive electrode
epss_neg	0.471	Solid phase vol-fraction negative electrode
epss_pos	0.297	Electrode phase volume fraction, positive electrode
i_1C	17.5 A/m <sup>2</sup>	1C discharge current
i0_neg_ref	1.1 A/m <sup>2</sup>	Exchange current density at reference conditions, negative electrode
i0_pos_ref	0.8 A/m <sup>2</sup>	Exchange current density at reference conditions, positive electrode
k_neg	8.7106E-10 m/s	Rate constant, negative electrode
k_pos	9.6422E-10 m/s	Rate constant, positive electrode
Ks_neg	100 S/m	Solid phase conductivity negative electrode
L_neg	1E-4 m	Length of negative electrode
L_pos	1.74E-4 m	Length of positive electrode
L_sep	5.2E-5 m	Length of separator
rp_neg	1.25E-5 m	Particle radius negative electrode
rp_pos	8E-6 m	Particle radius positive electrode
t_charge_stop	2000 s	Charge duration
t_disch_stop	2000 s	Discharge duration
t_ocp	300 s	Open circuit duration

## Appendix 2

Symbols in order of appearance

Electrochemical model states, inputs, outputs	
$c_s^\pm$	Lithium concentration in solid phase [mol/m <sup>3</sup> ]
$c_e$	Lithium concentration in electrolyte phase [mol/m <sup>3</sup> ]
$\phi_s^\pm$	Solid electric potential [V]
$\phi_e$	Electrolyte electric potential [V]
$i_e^\pm$	Ionic current [A/m <sup>2</sup> ]
$j_n^\pm$	Molar ion flux [mol/m <sup>2</sup> -s]
$i_0^\pm$	Exchange current density [A/m <sup>2</sup> ]
$\eta^\pm$	Overpotential [V]
$c_{ss}^\pm$	Lithium concentration at solid particle surface [mol/m <sup>3</sup> ]
$\theta^\pm$	Normalized surface concentration $c_{ss}^\pm / c_{s,\max}^\pm$ [-]
$I$	Applied current [A/m <sup>2</sup> ]
$V$	Terminal voltage [V]
Electrochemical model parameters	
$D_s^\pm, D_e$	Diffusivity of solid, electrolyte phase [m <sup>2</sup> /s]
$t_c^0$	Transference number [-]
$\varepsilon_s^\pm, \varepsilon_e$	Volume fraction of solid, electrolyte phase [-]
$F$	Faraday's constant [C/mol]
$\sigma^\pm$	Conductivity of solid [1/Ω-m]
$\kappa$	Conductivity of electrolyte [1/Ω-m]
$R$	Universal gas constant [J/mol-K]
$T$	Temperature [K]
$f_c/a$	Mean molar activity coefficient in electrolyte [-]
$a^\pm$	Specific interfacial surface area [m <sup>2</sup> /m <sup>3</sup> ]
$\alpha_a, \alpha_c$	Anodic, cathodic charge transfer coefficient [-]
$k^\pm$	Kinetic reaction rate [(A/m <sup>2</sup> )(mol <sup>3</sup> /mol) <sup>(1+α)</sup> ]
$c_{s,\max}^\pm$	Maximum concentration of solid material [mol/m <sup>3</sup> ]
$U^\pm$	Open circuit potential of solid material [V]
$R_f^\pm$	Solid-electrolyte interphase filme resistance [Ω-m <sup>2</sup> ]
$R_s^\pm$	Particle radius in solid phase [m]
$L^j$	Length of region $j \in \{-, \text{sep}, +\}$
Observer analysis / design parameters	
$n_{Li,s}, n_{Li,e}$	Total moles of lithium in solid, electrolyte phase [mol]
$\lambda$	Cathode estimation error system parameter
$p^\pm(r), p_0^\pm$	Cathode / anode observer gains
$\hat{c}_{ss}^\pm$	Estimated cathode surface concentration [mol/m <sup>3</sup> ]
$\tilde{c}_{ss}^\pm$	Processed cathode surface concentration [mol/m <sup>3</sup> ]
$\gamma$	Output inversion gain