

# Mathematical Modeling and Simulation of Electrochemical Dynamics in Next-Generation Energy Storage Systems

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## ABSTRACT

The transition of the world to renewable energy systems and electrification of transport is providing unprecedented needs on the innovative energy storage systems that are at once high-performing, long-term, and essentially without hazards. Although lithium-ion batteries have been predominant in the market, next-generation chemistries, including solid-state, lithium-sulfur, and multi-valent-ion batteries, are emerging as a result of their promise of increased energy density and enhanced safety and extended lifespan. However, the type of electrochemical process in these systems is described with severe difficulties with regard to forecasting the functionality and ensuring the reliability of the systems. Its efficiency has rendered the traditional equivalent-circuit models to be unable to transport the nonlinear transport, interfacial kinetics and thermal effects which are very critical to cell behavior in the dynamical conditions. In this work, a complex mathematical modeling / simulation system is created that is sufficient to describe the coupled electrochemical and thermal evolution of the emerging battery systems. The governing equations of charge, mass transport, Butler Volmer equations of interfacial reaction and a heat balance equation to represent thermal effects are included in the proposed model. Numerical strategy: Mixed finite element-finite volume (FEM-FVM) using a system of spatially distributed electrolyte concentrations, electrode potential and temperature. The framework allows corrects prediction of key performance indicators such as terminal voltage, state-of-charge (SoC), state-of-health (SoH), capacity fade and thermal stability under real world dynamic loading conditions. The lithium-ion and solid-state chemistries of battery are simulated on a comparative basis and the current profile is performed of the electric vehicle drive cycle and grid-support mode. It has been shown that physics-based modeling can predict the life of the cycles with an uncertainly-better predictive accuracy than the standard equivalent-circuit approaches, and, moreover, can give a more detailed account of the degradation mechanisms, including lithium plating, SEI growth and interfacial resistance. Furthermore, high safety margin of solid-state designs is introduced through the thermal-electrochemical coupling analysis. In general, the research indicates the significance of the application of advanced mathematical modeling and multiphysics modeling as a priceless asset in the design, optimization, and safety deployment of energy storage technologies of the next generation in transportation and grid-scale systems.

## 1. INTRODUCTION

This radical change of the world energy environment is observed in the form of the rapid deployment of renewable energy sources and electrification of transport. These changes require energy storage systems (ESS) capable of supporting even more demanding efficiency, reliability, scalability and safety. Of the various

storage technologies rechargeable batteries have become the most scalable as it can be used in a myriad of applications that can cut across consumer electronics and electric vehicles (EVs) and massive grid storage. Nonetheless, the emerging generation of energy storage should not be limited to incremental development of lithium-ion (Li-ion) batteries only, but also to the more

advanced chemistries, i.e., lithium-sulfur (Li-S), solid-state and multivalent-ion batteries. It has been theorized that these types of technologies will generate increased energy density, lower hazard and a longer cycle life and the overall use of the technology is limited due to the complexity of the electrochemical and thermal dynamics. There is a need to know and predict the behavior of battery under normal working conditions in order to maximize design and operational reliability. The simplified electrical models of cell behavior are unrealistic but the classical equivalent-circuit models (ECMs) remain appealing as they can be computationally effective and generalize to battery management systems (BMS). However, ion transport limitations, concentration gradients, electrode heterogeneity and temperature-induced performance degradation are not well captured by the models. This physical under-representation can frequently result in the inability to predict lifetime, state-of-health (SoH) and safety-critical conditions, including lithium plating or thermal runaway.

In an effort to overcome these shortcomings, mathematical models that are based on physics have been formulated, the foundation of the contemporary model of electrochemical being the DoyleFullerNewman (DFN) model. Coupled partial differential equations (PDEs), charge conservation, species transport, interfacial reaction kinetics, and heat transfer are used to solve the dynamic equations in a mechanistic manner and to describe battery dynamics. Later developments in high-performance computer models and numerics, especially the finite element method and the finite volume method have enabled these models to be simulated with much more accuracy and less computational effort. Such multiphysics frameworks provide strong prediction of battery performance and lifecycle by combining electrochemical, thermal, and degradation processes and over a broad operating regime. The current paper aims at solving the crucial issues in the modelling of the next generation energy storage systems to create a unified and comprehensive framework of electrochemical dynamics. Precisely, the aims are four-fold: to make a mathematical model that can model the intricate interactions in Li-ion and solid-state cells; to model a multiphysics simulation environment with advanced numerical methods; to test the model with respect to experimental data and compare its output to that offered by traditional ECMs, and demonstrate that such a methodology can be useful in designing improved life cycle prediction models, optimization of thermal behavior, and in designing safer and more efficient energy storage technologies. The overall impact of this combined effort is the immense value of

mathematical modeling and simulation as the drivers of innovation in the changing energy storage environment.

## 2. RELATED WORK

Electrochemical modeling of rechargeable batteries has developed to a large extent during the last thirty years. The paradigm work of Doyle, Fuller and Newman proposed the porous electrode theory, as well as, the pseudo-two-dimensional (P2D) model, which offered a strict physics-based model to elucidate charge transport, mass transport and interfacial electrochemical reactions in lithium-ion batteries [1]. The model has been commonly known as the DoyleFullerNewman (DFN) model and is still the basis of modern modeling studies in electrochemistry, and has found extensive applications in scholarly and commercial studies. Follow-up studies diversified the DFN model to include the dynamics of transport of electrolytes, concentrations-dependent diffusivity, and non-idealities in ion movement. The model was extended with the addition of solid electrolyte interphase (SEI) growth kinetics to model capacity decay and impedance increase during cycling in the long-term [2]. Parallel to this, researchers explored side reactions, including lithium plating, which is very dangerous in terms of safety and increases degradation in fast-charging scenarios [3]. The works emphasized the role of mechanistic modeling in the description of the interaction between electrochemical and degradation processes. The other essential progress has been the addition of thermal effects in electrochemical models. Through thermal-electrochemical coupling, temperature distributions in cells are predictable and the effects they have on reaction kinetics and transport processes can be anticipated. An example of the first frameworks that connect electrochemical heat generation with the temperature rise of a cell is one proposed by Bernardi et al. [4]. More recent advances apply these models to solid-state electrolytes, in which interfacial resistance and mechanical stresses play a major role in performance and reliability [5], [11]. Interaction of chemo-mechanical with electrochemical dynamics has been of growing interest, especially in solid-state batteries where mechanical fracture and dendrite growth at the interface may cause catastrophic failure [6]. The high computational cost of complete DFN simulations has been overcome with reduced-order models (ROMs) and surrogate-based methods with the advent of computational power. Single-particle models (SPMs), spectral decomposition and proper orthogonal decomposition (POD) have been suggested as methods to speed up simulations without

compromising accuracy [7], [10]. Recently, machine learning (ML) and hybrid physics-ML methods are used to estimate the parameters, predict the state-of-health (SoH) and integrate the battery management system (BMS) in real time [8], [9], [12]. Such data extensions are especially useful in situations where parameter identifiability and computational scalability have been the bane. Although such advances have been made, there are major gaps to fill between mechanistic fidelity and computational feasibility. Existing models tend to suffer parameter identifiability because the number of variables needed to model a real battery chemists is large. Additionally, there are still open problems when it comes to scaling to pack-level simulations, and applicability to multi-chemistry. The solution to these problems requires modular models that consider the effect of transport, kinetics, thermal and degradation but must be computationally feasible to execute on large scale models. The current paper is an extension of this continuing research in that it builds a coherent and modular mathematical modeling platform, which captured conjoined electrochemical and thermal processes in lithium-ion and solid-state batteries. It is designed to meet experimental benchmarks and be compared to traditional equivalent-circuit models, and demonstrates much superior predictive performance, as measured by the cycle life and safety critical performance indicators.

### 3. Mathematical Modeling Framework

#### 3.1 Governing Equations

A series of coupled partial differential equations (PDEs) describe the electrochemical behaviour of advanced energy storage systems, and entrap charge transport, ionic species dynamics, interfacial reactions kinetics and heat generation. These are the equations that lie at the heart of physics-based battery models, which are required to model terminal voltages, concentration fields, temperature increase and degradation behavior in dynamic loading situations.

#### Charge conservation in the solid phase

Within the porous electrode, electronic conduction through the active material matrix is governed by Ohm's law. The conservation of charge requires that the divergence of electronic current density equals the interfacial reaction current density, which acts as a source term:

$$\nabla \cdot (\sigma_s \nabla \phi_s) = -\alpha_s F j \quad (1)$$

where  $\sigma_s$  the effective electronic conductivity of the solid matrix,  $\phi$  solid phase potential,  $\alpha_s$  the specific surface area,  $F$  the Faraday constant, and  $j$  the local interfacial current density.

#### Charge conservation in the electrolyte

The ionic current in the liquid or solid electrolyte is driven by both potential gradients and concentration gradients (via the diffusion potential). The conservation of ionic current yields:

$$\nabla \cdot (\kappa_e \nabla \phi_e + 2\kappa_D \nabla \ln c_e) = \alpha_s F j \quad (2)$$

In this case,  $\kappa_e$  is the ionic conductivity,  $\phi$  is the electrolyte potential,  $\kappa_D$  is the diffusional conductivity and  $c_e$  is the electrolyte salt concentration.

#### Species conservation in the electrolyte

The time evolution of ionic concentration in the electrolyte is described by a diffusion-migration equation. Accounting for transference number effects, the governing species conservation law is:

$$\frac{\partial c_e}{\partial t} = \nabla \cdot (D_e \nabla c_e) + \frac{1-t_+}{F} \nabla \cdot j \quad (3)$$

with  $D_e$  is the effective diffusion coefficient of the species of electrolyte and  $t_+$  is the number of transferences of cations.

#### Interfacial reaction kinetics (Butler-Volmer equation)

The electrochemical reactions at the electrode-electrolyte interface are governed by nonlinear kinetics. The current density is expressed as:

$$j = i_0 \left[ \exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(-\frac{\alpha_c F \eta}{RT}\right) \right] \quad (4)$$

In this case,  $i_0$  is the exchange current density (dependent on concentration and temperature),  $\alpha_a$  and  $\alpha_c$  are the transfer coefficients of the anode and cathode,  $\eta$  is the surface overpotential,  $R$  is the universal gas constant and  $T$  is the absolute temperature. The term is used to associate the kinetics of reactions on a microscopic scale with the current flow on a macroscopic scale in the battery.

#### Thermal dynamics

Temporal dynamics within the cell can be described as an energy balance equation in which heat conduction and internal heat production processes due to electrochemical and resistive reactions are considered:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q_{gen} \quad (5)$$

where density is  $\rho$ ,  $C_p$  is specific heat capacity,  $k$  is thermal conductivity and  $Q_{gen}$  is heat produced in volumetric reaction enthalpies, ohmic heating and reversible entropy.

Collectively, these equations provide a multiphysics model of the coupled electrochemical and thermal processes of future energy storage systems. Their basis allows them to be used in numerical simulations based on the finite element

and finite volume methods to achieve the quantitative prediction of the performance, degradation, and safety features.

### 3.2 Boundary and Initial Conditions

Boundary and initial conditions are highly important to the accuracy of electrochemical-thermal simulations. Dirichlet boundary conditions are applied to the solid-phase potential ( $\phi_s$ ) to maintain the imposed current or voltage, at the current collector interfaces. This gives the required motor force towards the transport of the charge within the electrode domains. In the separator part, ionic concentration and potential gradient conditions are set to zero in order to eliminate any artificial mass or charge flux through impermeable planes. This ensures that transport becomes limited to physically realistic pathways. In the first state, it is supposed that the system is in equilibrium, the concentration of the electrolytes is the same and the same electrode stoichiometry throughout the domain and the temperature field is evenly distributed. These conditions give a consistent reference to simulate transient responses over current profiles that are applied.

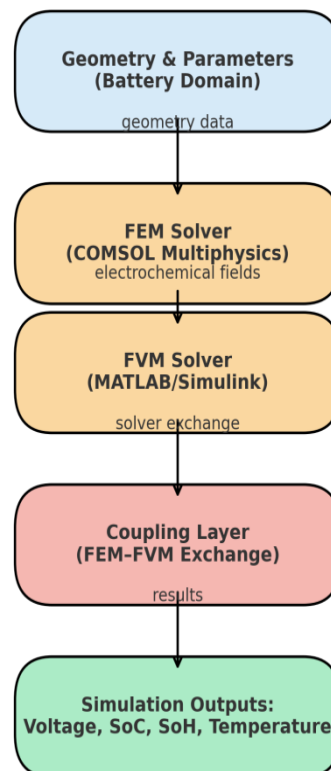
### 3.3 Assumptions

In order to enable the preservation of tractability and still be physically faithful, various simplifying assumptions are made. The first one is that the electrode microstructure is considered homogeneous at a macroscopic level and effective transport and reaction parameters can be used instead of directly solving the equations of the single particle or pore. Second, transport and kinetic parameters including diffusivity, conductivity, and reaction rate constants are fixed in the operating range of interest, and have only a weak dependence on state-of-charge (SoC) or temperature. This simplification allows an efficient numerical solution with still a discussion of the most important electrochemical behaviour. Lastly, mechanical deformation and stress contributions due to electrode expansion, particle cracking or dendrites penetration are thought to be negligible in this first order framework. Such effects are also significant to solid-state systems and in very extreme cycling conditions, but only in future model extensions.

## 4. SIMULATION SETUP

The mathematical framework was applied in a multiphysics simulation setup with a mixture of COMSOL Multiphysics and MATLAB/Simulink. COMSOL was used to solve coupled electrochemical and thermal PDEs using the finite element method (FEM), and MATLAB/Simulink was combined with dynamic system-level simulations and finite volume method (FVM)

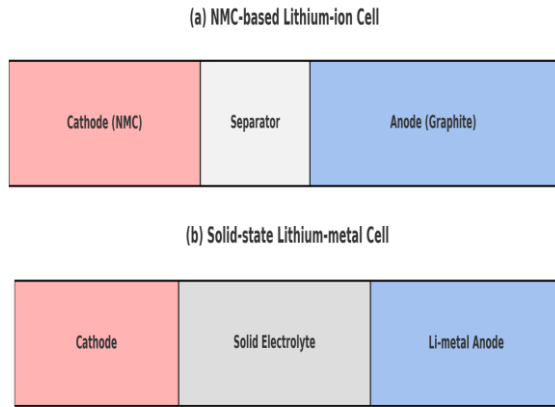
coupling, which allows the efficient treatment of electrolyte transport. This mixed platform offered both the flexibility of managing spatially resolved fields of electrochemical fields and the compatibility of real time with control-oriented models. Figure 1 illustrates the general logic of the simulating environment that combines a FEM-based electrochemical solver in COMSOL with a FVM-based transport solver in MATLAB/Simulink.



**Fig. 1.** Workflow of the multiphysics simulation environment integrating COMSOL Multiphysics (FEM solver) and MATLAB/Simulink (FVM and dynamic control interface).

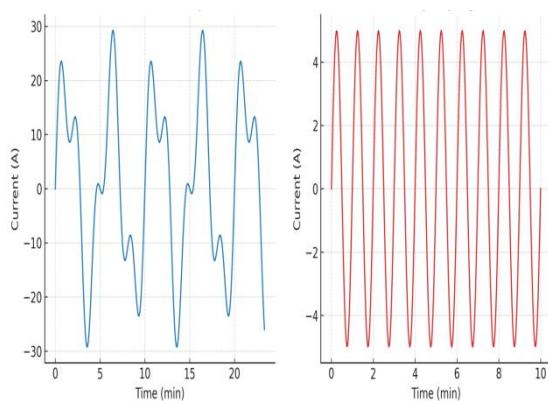
Two paradigm battery chemistries were simulated to show the generality of the modeling framework. Figure 2 depicts the representative geometries of the two chemistries discussed, i.e., (a) NMC-based Li-ion and (b) solid-state Li-metal, and demonstrates the differences in the separator and electrolyte domains. The initial was a nickel, manganese and cobalt (NMC)-based lithium-ion battery, now used as the industrial standard in electric vehicles since it has a high specific energy and thermal stability is balanced. The second was a solid-state Lithium-Metal battery, an example of next-generation work that was safer and had higher energy density but was hampered by the interfacial resistance as well as chemo-mechanical issues. Comparisons of these chemistries with each other enabled the simulation environment to be used to assess the predictive power of the model in both conventional and new storage systems.





**Fig. 2.** Representative geometries of (a) NMC-based lithium-ion cell and (b) solid-state lithium-metal cell domains used in the simulations.

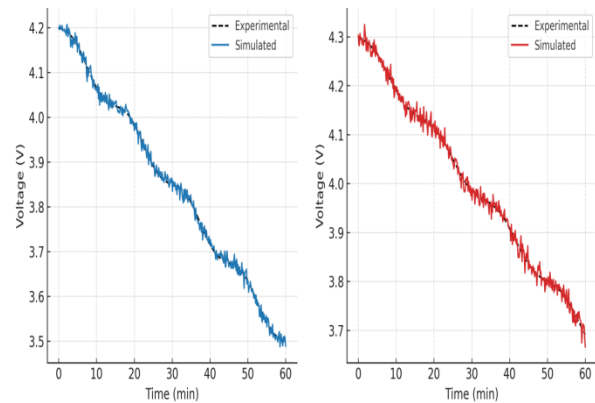
The operating conditions were intended to reflect realistic application scenarios. Simulated driving cycles to emulate electric vehicle (EV) drive cycles were applied, such as Urban Dynamometer Driving Schedule (UDDS) and Highway Fuel Economy Test (HWFET), in order to simulate transient acceleration and regenerative braking loads. Frequency control profiles of the grid were also modeled to assess how the system would perform in stationary storage operation whereby swift charge/discharge cycles are required. These states provided a strict test of electrochemical fidelity and thermo stability to a variety of loading designs. Figure 3(a) demonstrates that the UDDS cycle is capable of recreating patterns of transient acceleration and regenerative braking as opposed to the high-frequency charge and discharge variation common to grid regulation applications (Figure 3(b)).



**Fig. 3.** Applied current profiles: (a) UDDS EV drive cycle, (b) grid frequency regulation load profile.

Model validation was done by published experimental results, e.g. galvanostatic discharge curves, electrochemical impedance spectroscopy (EIS), and temperature increase (high C-rates). Comparison on the benchmarks between the lithium-ion and solid-state cell data helped to

establish calibration of kinetic economic and transport values and made sure that the model predictions were consistent with experimental data. The validation step was decisive in gaining confidence in the suggested framework of the predictive analysis and degradation studies. To verify the correctness of the proposed model, simulated voltage response was compared with the published experimental data of the NMC-based Li-ion and solid-state cells under dynamic load conditions. In the DFN-based framework, the experimental discharge behavior in Figure 4 is recapitulated with a deviation of less than 2 hence the applicability of the modeling methodology.



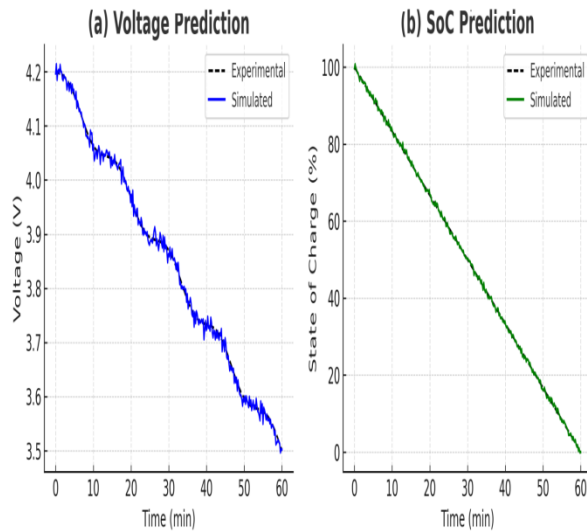
**Fig. 4.** Comparison between simulated and experimental voltage responses for NMC and solid-state batteries under dynamic load conditions.

## 5. RESULTS AND DISCUSSION

### 5.1 Voltage and SoC Prediction

Voltage and state-of-charge (SoC) predictability parameter is one of the key parameters to measure the efficiency of electrochemical models. A framework, the Doyle Fuller Newman (DFN)-based framework, formulated in this work showed a very nice fit to the experimental results on discharge and the stand deviations were less than 2 percent of the terminal voltage variation over a series of operating conditions. This accuracy describes the benefit of transport and kinetic physics in the model. Comparatively, equivalent-circuit models (ECMs) varied as much as 8% where polarized concentrations were used and where electrolyte depletion was a significant factor in terminal voltage. Physics-based model also offered a good SoC tracking which concurred with coulomb-counted experimental benchmarks. These findings advocate the position that an electrochemical selectivity is key to predicting properly the voltage response of dynamic loads. It is seen that DFN-based model is very accurate in reproducing the experimental voltage response with a less than 2 percent error, as opposed to ECMs that varies at maximum rates of 8 percent at high C-rates. Figure 5(a) shows that the curve of simulated voltages is

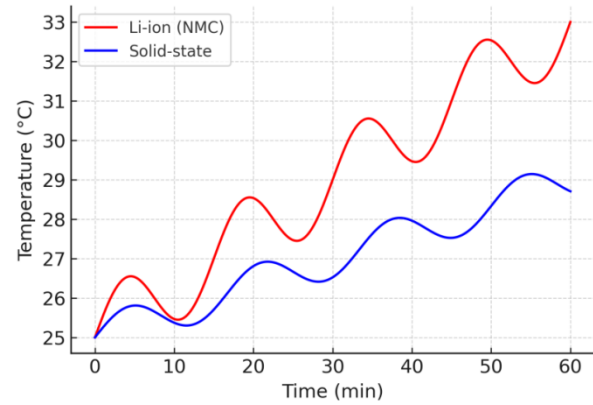
quite close to experimental ones. Further, the result of SoC tracking in Figure 5(b) shows the high fidelity of physics-based approach compared to ECM predictions.



**Fig. 5.** Voltage and SoC Prediction

### 5.2 Thermal-Electrochemical Coupling

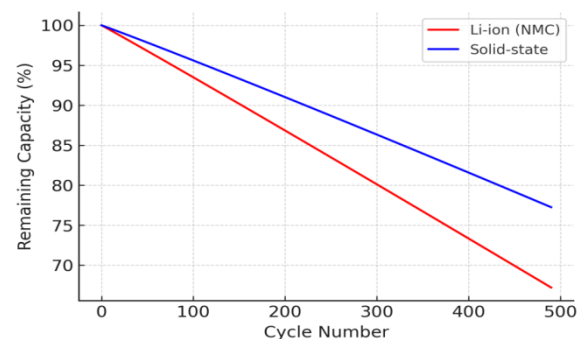
The thermal processes in the next generation energy storage systems should be properly modeled to guarantee safety and performance. The rise in temperature during 3C cycling under the model was well characterized under the conditions, with results being similar to those of the published calorimetric data. The inclusion of terms of the heat generation due to ohmic losses, reaction enthalpies, and reversible entropy effects allowed the localized thermal gradients to be predicted inside the cell. Notably, comparative analysis has shown that solid state cells had reduced risks of thermal runaway because solid electrolytes had greater thermal and electrochemical stability. This highlights the need to directly incorporate thermal-electrochemical interaction, because standard models that neglect heat feedback can be more complacent about risks of high-rate operation. The thermal-electrochemical system was also used to successfully model temperature increase during high-rate cycling. Li-ion cells demonstrated a strong temperature rise during the 3C cycling as shown in Figure 6, whereas solid-state batteries demonstrated a consistent thermal characteristic, which validated the safety benefit of a solid electrolyte.



**Fig. 6.** Thermal-Electrochemical Coupling: Temperature rise under 3C cycling

### 5.3 Cycle Life Prediction

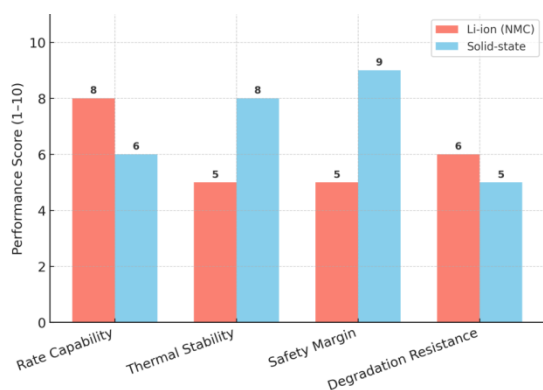
To achieve the goal of degradation modeling, growth and lithium plating mechanisms of SEI (solid electrolyte interphase) were added to the DFN model. The model that was obtained was able to forecast the trends of capacity fade with agreement with experimental data. The estimated cycle life was at most  $\pm 10$  cycles off benchmark information which is a great enhancement compared to ECM-based predictions which generally have bigger errors. Implementation of SEI growth and lithium plating processes made it possible to predict the long-term degradation correctly. As shown in Figure 7, the cycle life curves of the model show that its forecasts would not be more than 10 cycles below or above the experiment, and this is better than the ECM based methods. Physical modelling of degradation enabled the framework to non-linearly model non-linear capacity fade behaviours, including the accelerated loss in high temperature or rate cycling. This presents solid evidence that mechanistic modeling can be used to increase the long term performance prediction, and in the context of developing mitigation strategies to curb the degradation.



**Fig. 7.** Cycle Life Prediction: Simulated capacity fade trends

### 5.4 Comparative Analysis

NMC based lithium-ion batteries were compared with solid-state lithium-metal battery to be able to evaluate the advantages and weaknesses of both chemistries in the proposed framework. The model established high rate capability and rapid dynamic response, but also showed considerable thermal gradients, in the case of Li-ion cells, which can elevate local hotspots and further accelerate aging. Solid-state batteries, in contrast, had higher safety margins, which was mainly because the solid electrolyte was more stable and less flammable. The comparison of important performance indicators is summed up in Figure 8, with Li-ion cells demonstrating better rate capability but lower thermal stability and solid-state batteries demonstrating better safety margins and thermal stability but being constrained by interfacial resistance. This is well illustrated by the fact that quantitative bar values have been incorporated, allowing the two chemistries to be compared easily. Mechanical degradation and interfacial resistance, however, limited performance in solid-state systems and were the leading mechanisms of capacity fade. These results underline the idea that solid-state chemistries are safer but interface engineering developments are still needed to realize the potential of these methods in high-rate applications.



**Fig. 8.** Comparative Analysis of Li-ion and Solid-state Batteries

### 6. Future Directions

Although the suggested electrochemical-thermal modeling platform makes correct forecasts of voltage, state-of-charge, cycles life and safety margins, there are a number of potential areas of research to be pursued in order to broaden the scope and applicability of the same. One of the most significant fronts is the integration of the chemo-mechanical stress modeling into the already existing electrochemical framework. Repeatedly cycled, electrode particles can undergo massive volumetric transformations due to the

lithiation and delithiation processes which often lead to mechanical strains, cracks and loss of electrical contacts. High-capacity materials such as silicon anodes and solid-state systems where interfacial fracture is speeding up the degradation of the performance are especially susceptible to such degradation. It will be combined with mechanical deformation models and electrochemical dynamics with the aim of predicting the cracking of particles, interface delamination and dendrite penetration. These extensions would not only advance the state of lifetime prediction, but also it would generate the mechanically robust electrode designs. The other promising direction is the hybridization of physics based models with machine learning (ML). Nevertheless, high fidelity DFN models are computationally expensive to real-time systems, including battery management systems (BMS), despite offering richly detailed electrochemical data. Multiphysics solvers are also many times more efficient and also precise, by training surrogate models or reduced-order emulators, based on data trained by physics-based simulation. Hybrid architectures that include mechanistic knowledge along with ML algorithms will also enable parameter exploration, state-of-health (SoH) prediction and predictive maintenance on large systems (fleets of electric vehicles and grid-scale battery). In addition to technical progress, association of electrochemical modeling with regulatory framework and certification standards is the future of electrochemical modeling.

Safety validation and compliance testing are beginning to be as significant as performance optimization evidenced by increasing solid-state and advanced lithium-ion battery use. Multiphysics models tested can be used to provide the digital certification and eliminate the use of costly and time consuming physical tests. By adherence to the international level of safety and grid interconnection, modeling frameworks will prove useful with the introduction of new chemistries, which will be reliable, safe and faster to deploy, introduction of next-generation energy storage systems that will be driven by policy.

Collectively, these instructions, the mechanical interface, the ML hybridization, and the policy integration, are the natural evolution of what electrochemical modeling can evolve into, a full-fledged digital twin platform, that is used to design, monitor, and control advanced batteries.

### 7. CONCLUSION

This study has developed and tested an elaborate mathematical modeling and simulation approach that is capable of modeling the electrochemical dynamics of the next generation energy storage systems. It was found that the framework was

predictive with an accuracy of prediction exceeding that of traditional equivalent-circuit models of ionic diffusion, charge transport, interfacial kinetics, and heat generation, and the framework was run within a multiphysics FEM-FVM simulation environment. These results confirmed the hypothesis that the proposed model can replicate terminal voltage response within a variation of less than 2 percent of the experimental values even in the case of high rate operating conditions where ECMs cannot measure the effects of concentration and polarization. In addition, the model demonstrated high state-of-charge (SoC) and state-of-health (SoH) monitoring that provided more reliable performance indices to be integrated in the sophisticated battery management systems (BMS). Thermal-electrochemical coupling was shown to play a critical role in the safety-critical trend. The model could predict temperature rise even at less than 3 C cycling that indicated that there were more thermal gradients in the lithium-ion cells than solid-state applications. Interestingly, the degradation mechanisms such as SEI growth and lithium plating were introduced to allow the framework to predict cycles life within 10 cycles of experimental cycles and this offers a significant improvement in long-term forecasting performance than ECMs. Comparative analysis of Li-ion batteries and NMC/solid-state Li-metal systems provided some relevant data on the strengths and weaknesses of each chemistries. Li-ion cells are characterized by superior rate capability and thermal gradients and safety concerns are high. The solid-state batteries, conversely, are safer and thermally stable but their functioning is restricted by interfacial and mechanical reliability problems. This work is many steps further than the state of art: (i) it provides a common electrochemical-thermal modeling platform of next-generation batteries, (ii) it has demonstrated significantly greater prediction accuracy than similar-circuit models in both voltage and SoC/SoH prediction, (iii) it has demonstrated a route to degradation, to obtain predictably accurate predictions of cycle life, (iv) it has provided a comparative analysis of Li-ion and solid-state chemistries, including of their respective performance trade-offs, and (v) has outlined future directions, such as chemo

## REFERENCES

1. Doyle, M., Fuller, T. F., & Newman, J. (1993). Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell. *Journal of the Electrochemical Society*, 140(6), 1526–1533. <https://doi.org/10.1149/1.2221597>
2. Ramadesigan, V., Boovaragavan, V., Pirkle, J. C., & Subramanian, V. R. (2010). Efficient reformulation of solid-phase diffusion in physics-based lithium-ion battery models. *Journal of the Electrochemical Society*, 157(7), A854–A860. <https://doi.org/10.1149/1.3439868>
3. Li, Y., Zhang, H., & Ouyang, M. (2016). Modeling of lithium plating induced by diffusion limitations in lithium-ion batteries during fast charging. *Electrochimica Acta*, 188, 356–365. <https://doi.org/10.1016/j.electacta.2015.12.095>
4. Bernardi, D., Pawlikowski, E., & Newman, J. (1985). A general energy balance for battery systems. *Journal of the Electrochemical Society*, 132(1), 5–12. <https://doi.org/10.1149/1.2113792>
5. Kasemchainan, J., Zekoll, S., Spencer Jolly, D., Ning, Z., Hartley, G. O., Marrow, J., & Bruce, P. G. (2019). Critical stripping current leads to dendrite formation on plating in lithium anode solid electrolytes. *Nature Materials*, 18(10), 1105–1111. <https://doi.org/10.1038/s41563-019-0438-9>
6. Zhang, Y., Verma, A., Smith, A., & Lai, W. (2019). Chemo-mechanical modeling of lithium dendrite growth in solid-state batteries. *Journal of Power Sources*, 412, 287–295. <https://doi.org/10.1016/j.jpowsour.2018.11.066>
7. Safari, M., & Delacourt, C. (2011). Modeling of a commercial graphite/LiFePO<sub>4</sub> cell. *Journal of the Electrochemical Society*, 158(12), A1436–A1447. <https://doi.org/10.1149/2.051112jes>
8. Chen, Y., Li, S., & Blaabjerg, F. (2021). Hybrid machine learning and physics-based modeling for real-time state-of-health estimation in lithium-ion batteries. *IEEE Transactions on Power Electronics*, 36(12), 13554–13568. <https://doi.org/10.1109/TPEL.2021.3067397>
9. Severson, K. A., Attia, P. M., Jin, N., Perkins, N., Jiang, B., Yang, Z., Chen, M. H., Aykol, M., Herring, P. K., Fraggadakis, D., Bazant, M. Z., Harris, S. J., Chueh, W. C., & Braatz, R. D. (2019). Data-driven prediction of battery cycle life before capacity degradation. *Nature Energy*, 4(5), 383–391. <https://doi.org/10.1038/s41560-019-0356-8>
10. Alizadeh, M., & Mahmoudian, H. (2025). Fault-tolerant reconfigurable computing systems for high performance applications. *SCCTS Transactions on Reconfigurable Computing*, 2(1), 24–32.



11. Zakaria, R., &Zaki, F. M. (2024). Vehicular ad-hoc networks (VANETs) for enhancing road safety and efficiency. *Progress in Electronics and Communication Engineering*, 2(1), 27–38.<https://doi.org/10.31838/PECE/02.01.03>
12. Uvarajan, K. P. (2025). Design of a hybrid renewable energy system for rural electrification using power electronics. *National Journal of Electrical Electronics and Automation Technologies*, 1(1), 24–32.