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Highlights

- A systematic review on control-oriented battery electrochemical models is proposed.
- P2D model and various order-reduction techniques are investigated.
- Enhanced multi-particle, multi-scale, ageing, and thermal models are explored.
- Different parameterization methods for electrochemical models are summarized.
- Future trends, challenges and suggestions are discussed.

Electrochemical modeling and parameterization towards control-oriented management of lithium-ion batteries

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Abstract

Battery management systems based on electrochemical models could achieve more accurate state estimations and efficient battery controls with access to cell unmeasurable physical variables. As battery electrochemical models are governed by first-principle partial differential equation sets, model complexity and multiple parameter determination are bottlenecks for their wider applications. This paper gives a systematical review of recent advancements in electrochemical model development and parameterization. Specifically, classic pseudo-two-dimensional model and related model order reduction methodologies are first summarized and analyzed. Given that the homogenization hypothesis of the pseudo-two-dimensional model could lead to significant model mismatch under some operational conditions, enhanced models considering cell internal inhomogeneity with multi-particles, multi-scales, ageing and thermal dynamics are examined. To facilitate model portability, parameter identification techniques of these models are classified, and solutions for optimizing the parameterization procedure are explored. Finally, current research gaps in the literature and remaining challenges are discussed and highlighted with some suggestions. This review will therefore inform the engineers of battery management and control engineering, whilst boosting the research, design and operation of control-oriented electrochemical models for smarter battery management at different readiness levels.

Keywords: Lithium-ion battery, Control-oriented management, Energy storage, Electrochemical model, Model reduction, Parameter identification

Abbreviations

EV	Electric vehicle
P2D	Pseudo-two-dimensional
BMS	Battery management system
PDE	Partial differential equation
SPM	Single particle model

SPMe	Single particle model with electrolyte dynamics
CCCV	Constant-current constant-voltage
DAE	Differential algebraic equation
MPM	Many particle model
DFN	Doyle-Fuller-Newman
FVM	Finite volume method
LFP	$LiFePO_4$
SOC	State of charge
ECM	Equivalent circuit model
IMA	Integral method approximation
DRA	Discrete-time realization algorithm
PSD	Particle size distribution
ROM	Reduced order model
SEI	Solid electrolyte interphase
EIS	Electrochemical impedance spectroscopy
GITT	Galvanostatic intermittent titration technique

1. Introduction

Clean, renewable energy sources are needed to help create a sustainable society. Due to the superiorities in terms of energy density, efficiency, low discharge rate, and environmental friendliness [1, 2], lithium-ion (Li-ion) batteries have become one of mainstream energy storage components in numerous sustainable applications such as electric vehicles (EVs) [3, 4], renewable energy storage, and smart grid [5].

Battery management systems (BMSs) generally implement model-based algorithms to protect battery from abuse, prolong battery service life, and maintain battery operated in an efficient status [6, 7]. As a key functional part for achieving control-oriented battery management, Li-ion battery modeling techniques with a specific form can be mainly divided into two categories: equivalent circuit models (ECMs) and electrochemical models.

For the ECMs [8, 9], one or more parallel resistor-capacitor sub-circuits are applied to perform phenomenological emulations of cell external responses, where battery current, voltage and ageing behavior could be also well matched [10, 11]. Due to the simple structure and low computational burden, ECMs have been widely adopted in BMSs for control-oriented management [12, 13, 14]. In contrast, electrochemical models allow the enhanced monitoring and prediction of battery individual mechanisms [15]. Given the capability of capturing cell-intrinsic physical states, electrochemical model-based BMSs enable health-aware control of Li-ion batteries to improve their operational safety, reliability, and efficiency [16, 17, 18]. However, the electrochemical models generally consist of a series of partial differential equations (PDEs), which would inevitably increase the computational complexity in battery practical applications [19]. As the most widely-adopted electrochemical model, battery pseudo-two-dimensional (P2D) model is derived from the porous electrode theory, concentrated solution theory, and kinetics equations [20]. The P2D model is established using the volume averaging technique and treats the electrode as a homogeneous medium [21], where the full order P2D model is computationally expensive and difficult to be implemented on the hardware. Therefore, it is necessary to simplify the P2D model before the control-oriented applications can be realized.

To reduce computational complexity of electrochemical models, various simplified versions of the P2D model have been investigated. To be specific, by simplifying each electrode as a single solid spherical particle, single particle model (SPM) becomes the most popular simplified P2D model [22]. However, due to electrolyte concentration and potential are considered to be constant for the cell, the performance of SPM can only match as well as the rigorous P2D model in the cases where the current rate is less than 1C. To overcome this limitation, both electrolyte are temperature dynamics are integrated with SPM [23], where the acceptable accuracy and low-cost computational effort enable these SPMs become competent for developing battery state estimation strategies [24] and optimal control approaches [25]. Another promising approach is to linearize the coupled PDEs of rigorous P2D porous electrode and develop analytic Laplace-domain transfer functions from the linearized model [26]. For example, the transfer functions of reation flux, solid-electrolyte potential difference, overpotential, and solid particle surface concentration versus input current were derived [27]. Then a low-order model was generated through a residue-grouping approach. A novel discrete-time realization algorithm (DRA) was used to produce a reduced-order discrete-time state-space model [28]. Some researchers also use Padé approximation to match the frequency responses of PDEs [29]. Furthermore, the polynomial profiles (PP) are fast approximations of electrolyte concentration and potential along the x direction [30], while the solid-phase diffusion along the r direction [31]. The PP model poses simple structure and converts PDEs into the Differential Algebraic Equations (DAEs). The spatial discretization methods including the finite difference [32] and finite volume method [33], are effective tools for numerical solutions of PDEs [34]. The discretization methods could achieve high accuracy because they divide the feasible region into multiple cells [35]. Some researchers combine the ECM and electrochemical models to make best of the two approaches, e.g. high computational speed with physical meaning [36]. A recent trend of research is to use the asymptotic techniques for achieving the order reduction of the electrochemical model [37]. The asymptotic reduction approach is based on exploiting the vastly different time scales of various physical processes, leading to a more organic simplification [38].

On the other hand, P2D model is formulated under the homogeneity assumptions. For example, the P2D model assumes that the active material particles are spherical and distribute uniformly with identical radius [39]. However, practical electrodes have non-spherical particle shapes that exhibit large dispersity [40]. This indicates that the P2D model would be limited in the cases where cells have dispersed particle shapes. Therefore, the accuracy of P2D model would be degraded in predicting cell voltage under extreme circumstances, such as low SOC range, resting period [41], and high temperatures [42]. In addition, volume average approach does not consider the actual topology and electrode morphology [43]. Porosity and active volume fraction are not constant throughout battery lifespan due to the volume changes, cracks, lithium plating and stress effects occurring in the electrodes during cell charge and discharge [44]. The lithiation/delithiation mechanisms describing the intra-particle phase transformation of P2D model fail to analyze the coexistence of Li-poor phase and Li-rich phase within LFP crystals [45]. The coexistence of two phases is the major cause of the flat open-circuit-potential within LFP electrodes [46]. Therefore, it can be inferred that the limitations of the P2D model arise from the model simplification process. Many researchers have extended P2D model to consider the inhomogeneity of particle and electrode [47]. A simplified electrochemical multi-particle

Table 1: An overview of the published literature related to battery electrochemical models.

Topic	Reference	Content
P2D model simplification	[60]	Simplified P2D models.
	[61]	P2D model order reduction techniques.
Enhanced electrochemical model	[62]	Multiscale Lithium-ion battery modeling from materials to cells.
	[63]	Multiscale modeling of rechargeable batteries.
Parameter identification method	[58]	Post-mortem analysis of lithium-ion batteries.
	[64]	Computational parameter estimation methods.
	[65]	Battery testing and experimental datasets.
	[66]	Summarization of methods to measure or infer parameters.

model for LFP cathodes in Li-ion batteries was developed [48]. Therein, the active material particles of non-uniform properties (e.g., size, contact resistance, material chemistry etc.) were incorporated. The multi-particle model could accurately simulate the cell charge/discharge current rates up to 5C. The realistic 3D anode structures using a stochastic microstructure model was generated, which is parameterized using tomography data. The results show that the deviations between uniform and realistic electrodes are pronounced at high current rates [49]. Multiple cases of heterogeneities, such as non-uniform ionic resistance and active material loading, are studied at different charge and discharge current rates [50]. The results indicate that higher current rates increase the non-uniformities of temperature, current density, positive and negative electrode SOC, especially in the case of charging [39].

Accurate model parameterization is also crucial for efficient and reliable electrochemical model-based prediction, state estimation, and control [51]. Generally, there are two main solutions for identifying parameters of electrochemical models: direct measurements and invasive parameter estimations. For the direct measurement, after dismantling battery cell, its internal structures, compositions, and properties would be analyzed with specific instruments [52]. This type of solution is robust as the physical parameters of battery can be directly measured. A detailed review for the post-mortem techniques and subsequent electrochemical analysis of cell performance and physical-chemical properties can be found in [53] and [54], respectively. The invasive parameter estimation refers to the methods that estimate model parameters by fitting electrochemical model output to the measured cell quantities (e.g., terminal voltage, temperature) [55]. Due to most of the parameters are weakly correlated with the battery terminal voltage, complete set of parameters is difficult to be identified simultaneously [56]. Therefore, a stepwise solution is generally adopted to identify these parameters [57]. Both these two parameterization methods have their own merits and drawbacks. Cell postmortem analysis could provide visualized insights into material properties. However, this method is time-consuming and the related equipment used in the analysis is often expensive [58]. Parameter estimation method could save identification time but the robustness as well as validity of the estimated parameters need to be further verified [59].

To date, a few review articles regarding the battery P2D model simplification, enhanced electrochemical model, and parameter identification method are presented, as summarized in Table 1. It should be known that all these reviews mainly focus on one aspect alone. As battery electrochemical model towards control-oriented management generally requires to conduct all of the following steps, namely model simplification, improvement, and parameter identification, where these aspects are heavily correlated. In this context, a review article covering all these aspects is urgently required especially for promoting battery electrochemical model-based control applications. Here, a systematical review of electrochemical modeling and parameterization methods towards control-oriented management of Li-ion batteries is given, while their challenges and prospects are also discussed. The review is targeted to inform control-oriented technology choices and academic research agendas alike, thus advancing battery electrochemical model development at different technology readiness levels. The following topics are covered as:

- In Section 2, typical battery P2D model with different simplification solutions are comprehensively reviewed. Their merits and drawbacks are also thoroughly compared and discussed.
- For the enhanced electrochemical modeling technology, battery multi-particle model, electrochemical model with multiple scales, electrochemical model with ageing and thermal effects are reviewed in Section 3, and their advantages and disadvantages are discussed.
- For the parameterization of battery electrochemical model, technologies including physical parameter measurements and noninvasive parameter estimation are comprehensively surveyed in Section 4.
- Current research challenges are discussed in Section 5. Feasible solutions to address these challenges are suggested as future research direction towards the improvement of battery control-oriented electrochemical modeling technologies.

2. P2D model and simplifications

The pseudo-2-dimension (P2D) model pioneered by Doyle et al. is one of the most popular electrochemical models for Li-ion batteries [67, 68]. This type of model consists of numerous PDEs and is computationally complex for control-oriented applications [69], where various model reduction techniques are required to simplify P2D model. In this section, the development of rigorous P2D model is first introduced, followed by the summary and comparison of various P2D model order reduction methods and their control-oriented applications.

2.1. Definitions and derivations of the basic P2D model

P2D model is a classical electrochemical model and has been widely investigated. For the macroscopic model of Li-ion batteries, concentrated solution theory is generally utilized to describe the transport properties in the solution phase, while porous electrode theory is adopted to analyze the composite electrodes [70]. Here the concentrated solution theory assumes that electrolyte consists of a binary salt system (Li^+ and X^-) in a single solvent. For the porous electrode theory, a solution phase, a solid active-material phase, and any conductive filler or binding additives are considered as superimposed continua, hence all points of the electrode are perfectly connected. The active material is supposed to be comprised of multiple spherical particles with a diameter $R_{s,k}$ ($k \in n = negativeelectrode, p = positiveelectrode$). Based upon above assumptions, the P2D model could be established, as shown in Fig. 1. To be specific, the spherical electrode particles are defined in the domain $0 \leq r \leq R_{s,k}$. The electrolyte traverses across the two porous electrodes and separator ($0 \leq x \leq L$), where the anode, separator and cathode are defined in $0 \leq x \leq L_n, L_n \leq x \leq L_n + L_m$, and $L_n + L_m \leq x \leq L_n + L_m + L_p$, respectively. Here the subscripts n, m, and p denote the variables in negative electrode, separator, and positive electrode, respectively. The Li^+ diffusion in the solid particles with boundary conditions follows Fick's second law as [71]:

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial c_s}{\partial r}) \tag{1}$$

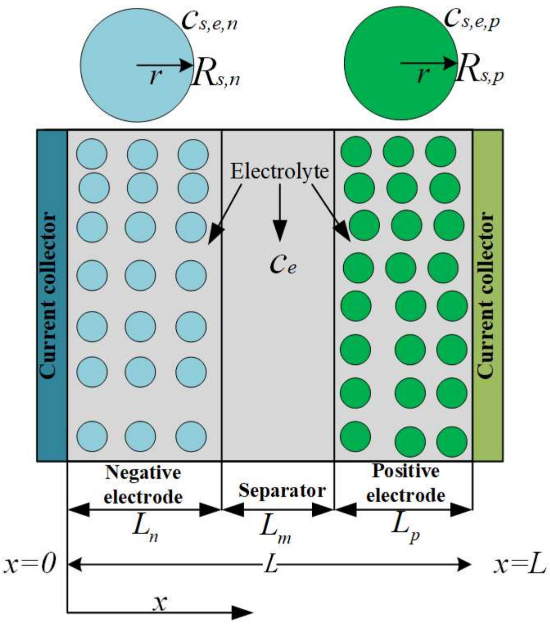

Figure 1: Schematic diagram of Li-ion battery P2D model.

$$\left.\frac{\partial c_s}{\partial r}\right|_{r=0} = 0, D_s \left.\frac{\partial c_s}{\partial r}\right|_{r=R_s} = -\frac{j}{a_s F} \tag{2}$$

where c_s is the solid concentration, j denotes the lithium flux across the boundary of solid phase, D_s is the solid diffusion coefficient, a_s is the specific interfacial area, R_s is the particle radius, and F is the Faraday constant. The lithium concentration at particle surface is denoted as $c_{s,e}$.

The solid electrode potential ϕ_s is described by the Ohm's law as [72]:

$$\sigma^{eff} \frac{\partial^2 \phi_s}{\partial x^2} - a_s j = 0 \tag{3}$$

where σ^{eff} is the effective electrode conductivity, a_s is the electrode specific surface area. The concentration of electrolyte is determined by [72]:

$$\varepsilon_e \frac{\partial c_e}{\partial t} = D_e^{eff} \frac{\partial^2 c_e}{\partial x^2} + \frac{a_s \left(1 - t_+^0\right)}{F} j \tag{4}$$

with the following boundary conditions:

$$\begin{bmatrix} \left.\frac{\partial c_e}{\partial x}\right|_{x=0} = 0, \left.\frac{\partial c_e}{\partial x}\right|_{x=L} = 0 \\ c_e(L_n^-) = c_e(L_n^+) \\ c_e((L_n + L_m)^-) = c_e((L_n + L_m)^+) \\ D_{e,n}^{eff} \frac{\partial c_e(L_n^-)}{\partial x} = D_{e,m}^{eff} \frac{\partial c_e(L_n^+)}{\partial x} \\ D_{e,m}^{eff} \frac{\partial c_e((L_n + L_m)^-)}{\partial x} = D_{e,p}^{eff} \frac{\partial c_e((L_n + L_m)^+)}{\partial x} \end{bmatrix} \tag{5}$$

where c_e denotes the electrolyte concentration, D_e^{eff} is the effective electrolyte diffusion coefficient as $D_e^{eff} = D_e \varepsilon_e^{brug}$. ε_e represents the volume fraction of electrolyte, and t_+^0 is the transference number of Li^+. Bruggeman coefficient is denoted as $brug$. The charge conservation in the electrolyte can be described by [73]:

$$\kappa^{eff} \frac{\partial^2 \phi_e}{\partial x^2} + \kappa_D^{eff} \frac{\partial^2 \ln c_e}{\partial x^2} + a_s F j = 0 \tag{6}$$

where ϕ_e is the electrolyte phase potential, κ^{eff} is the effective ionic conductivity as $\kappa^{eff} = \kappa \varepsilon_e^{eff}$, and κ_D^{eff} is a short term for $\kappa_D^{eff} = 2RT\kappa(t_0^+ - 1)/F$. Here the boundary conditions at two current collectors are:

$$\left.\frac{\partial \phi_e}{\partial x}\right|_{x=0} = 0, \left.\frac{\partial \phi_e}{\partial x}\right|_{x=L} = 0 \tag{7}$$

The lithium insertion process in the porous electrode is described by Butler-Volmer equation as:

$$j = i_0 \left(\exp\left(\frac{\alpha_a F}{RT}\eta\right) - \exp\left(-\frac{\alpha_c F}{RT}\eta\right) \right) \tag{8}$$

where i_0 is the exchange current density, $i_0 = Fk(c_e)^{\alpha_a}(c_{s,max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c}$, k is a kinetic rate constant. η is overpotential, which is an extra force required to overcome the surface reaction as :

$$\eta_k = \phi_{s,k} - \phi_{e,k} - U_{ocp,k}, k \in \{n, p\} \tag{9}$$

where U_{ocp} is the electrode open circuit potential and can be described by lithium surface concentration $c_{s,e}$. Cell voltage could be described by the potential difference between the positive and negative current-collectors, and voltage drop due to film resistance as [74]:

$$V(t) = \phi_s(L, t) - \phi_s(0, t) - R_f I \tag{10}$$

where R_f is the film resistance.

It should be known that the coupled PDEs (1)-(7) can be utilized to investigate battery electrochemical mechanisms and optimize battery designs without numerous experimental data. These PDE models are infinite–orders since there are infinite number of $x-$ and $r-$ dimensional variables to be calculated at each point in time t. A complete analytical solution of the governing PDEs is generally difficult to obtain. As the P2D models are too complicated to be implemented in real-time applications particular for battery control-oriented management, a great deal of efforts have been done to reduce the finite order of PDE models into small order while retaining fidelity, further resulting in the PDEs can be transformed into ordinary differential equations (ODEs) with relatively lower computational complexity.

The aim of developing simplified P2D models is to approximate the rigorous P2D models at a high accuracy but with a relatively low computational burden [75]. Battery management systems with the simplified P2D models have significant advantages over ECMs as this type of control-oriented models could provide richer electrochemical information, further benefitting cell optimal control, online estimation, optimization, and fault diagnostics [76].

2.1.1. Single particle model based

Single particle model (SPM) is a classical simplified version of the P2D model based on three critical hypotheses: First, the negative and positive electrodes are represented with only two spherical particles. Second, the electrolyte concentration and potentials are neglected. Third, the lithium flux is proportional to the input current. The SPM is computational efficient and could be adopted in control-oriented applications [77], as shown in Fig. 2. However, SPM would fail under the high current rates ($> 1C$) [78]. To further handle this limitation, some efforts have been made to improve SPM by considering the electrolyte [79] and thermal dynamics [80]. As a result, these enhanced SPMs are able to provide sufficiently accurate results under high current rates and achieve a substantially lower computational burden than P2D model [81].

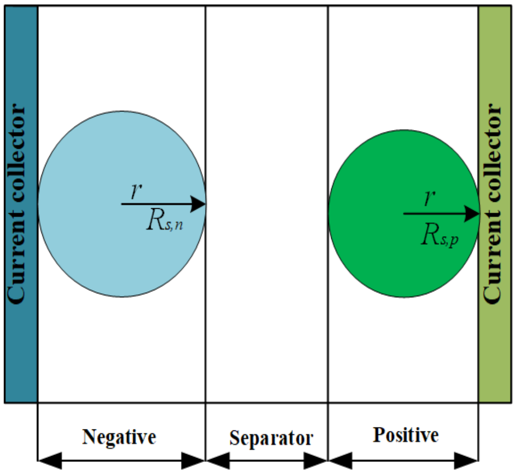

Figure 2: Schematic diagram of single-particle model.

2.1.2. Transfer-functions type

Besides, establishing transfer functions of all electrochemical variables and converting these transfer functions into low-order high-fidelity state-space approximate models is also becoming a promising solution to simplify the P2D model. This transfer-function-based solution can solve any subset of the internal electrochemical variables desired at any selection of internal cell locations. Even though it is mathematically complex to derive transfer functions, the final computational complexity could become as significantly low as the battery ECM [82].

The transfer functions for solid surface concentration, lithium flux and phase potential difference were first derived [83].With these transfer functions, model reduction techniques, including the truncated Taylor-series expansion, residue grouping, and nonlinear optimization were applied to generate a low-order electrochemical model. Here the terminal voltage from a 12th order state variable model could reach less than 1% error for pulse and constant current profiles at the current rates up to 50C. The state equation was constructed with constant negative real eigenvalues distributed in the frequency range from 0 to 10 Hz (15). This type of method was further extended to derive transfer functions for electrolyte concentration, solid and electrolyte potentials [84]. The reaction flux transfer function was given by:

$$\frac{J(z,s)}{I(s)} = \pm\upsilon^k(s)\frac{\sigma_k^{eff}\cosh(\upsilon^k(s)z) + \kappa_k^{eff}\cosh(\upsilon^k(s)(z-1))}{a_s^k F L_k A(\kappa_k^{eff} + \sigma_k^{eff})\sinh(\upsilon^k(s))} \tag{11}$$

where $k \in n$(negative electrode), p(positive electrode), $z = x/L_k$, ν is the unitless impedance ratio. Afterwards, the discrete-time realization algorithm (DRA) was used to convert these transfer functions into an optimal low-order discrete-time state-space approximate model.

It should be noted that the following critical assumptions are made for both Smith and Plett's work when solving the transfer functions from nonlinear PDEs: First, the nonlinear equations could be linearized by using Taylor series. This assumption is reasonable as the transfer functions only exist for linear systems. Second, the electrolyte potential ϕ_e is predominantly a function of lithium flux j, further indicating that the effect of electrolyte concentration on the electrolyte potential was ignored. However, the second assumption could fail when the battery cell is operated under constant-current conditions, where a large concentration gradient occurs in the electrolyte. Through eliminating the requirement of using second assumption, a more complicated transfer functions for PDEs [85] was observed. Similarly, DRA method was employed to obtain the final reduced-order model whose computational complexity is similar to battery ECM.

The Padé approximation method is an effective tool for converting transcendental transfer functions (the exact solutions of diffusion equations) into polynomial transfer functions that can be easily deployed in control-oriented applications [86]. The Nth-order Padé approximation of a transcendental transfer function $G(s)$ is a ratio of two polynomials in s where the denominator is of order N. The numerator is of order N or less. Normally, the computational speed is determined by the denominator order as:

$$G(s) = \frac{\sum\limits_{m=0}^{M} b_m s^m}{1 + \sum\limits_{n=1}^{N} a_n s^n} (M \leq N) = \frac{num(s)}{den(s)} \tag{12}$$

where M is the order of numerator and N is the order of denominator. b_m and a_n are coefficients for the numerator and the denominator, respectively.

The Padé approximation of the transcendental transfer functions for the solid-state diffusion were applied [87], where the first-order, second-order, and third-order Padé approximations were presented and compared in the frequency domain. It turned out that the Padé approximates could also well capture the low-frequency dynamics, where the model would become more accurate at high-frequency as the Padé order increases.

$$\frac{\tilde{C}_{ss}(s)}{J(s)} = \frac{R_s}{FD_s} (\frac{\tanh(R_s \sqrt{^s/_{D_s}})}{\tanh(R_s \sqrt{^s/_{D_s}} - R_s \sqrt{^s/_{D_s}}}) \tag{13}$$

where R_s is the particle radius, F is the Faraday constant, D_s is the solid-phase diffusion coefficient.

A model-order reduction procedure based on the Padé approximation was presented [88]. The frequency distribution of current profiles concerning two regulatory driving cycles including the US06 highway cycle and Federal Urban Dynamometer Schedule (FUDS) was investigated. As 90% of these cycles are within the frequency domain less than 2.5 Hz, a first-order Padé approximation is therefore chosen to model the liquid diffusion dynamics, and a third-order truncation is selected for the solid-diffusion dynamics. Based upon the Lee's derivation of transcendental transfer functions on lithium flux j, solid surface concentration $c_{s,e}$, electrolyte concentration c_e, and electrolyte potential, a reduced-order model was presented where Padé approximates were used to handle the complicated transcendental transfer functions. The obtained reduced-order model is amenable with rapid computation for control-oriented applications [89].

Integral method approximation (IMA) is another effective solution to solve the transfer functions, where a distribution of the electrochemical variables across battery cell is assumed and the governing equations are integrated. The IMA was used to solve $Li+$ conservation across the anode, cathode, and separator of cell [90]. A parabolic distribution of the electrolyte concentration was assumed and substituted into Li^+ conservation equations, where the boundary conditions are integrated and simplified to obtain the third order transfer functions for electrolyte concentrations.

2.1.3. Polynomial expression

The polynomial profiles are simple approximations for solid-state concentration function [91] and electrolyte concentration distributions [92]. The efficient microscale diffusion inside porous electrodes was developed, assuming that the solid-state concentration inside spherical particle could be expressed as a polynomial in the spatial direction. The two-parameter and three-parameter parabolic models presented the following forms as:

$$\begin{aligned} C(z,\tau) &= a(\tau) + b(\tau)z^2; \\ C(z,\tau) &= a(\tau) + b(\tau)z^2 + c(\tau)z^4; \end{aligned} \tag{14}$$

The approximate models were tested for arbitrary functions of pore wall flux and could save computational effort by over 80% without compromising the accuracy [31]. The parabolic models was extended for higher charge-discharge rates [93]. Specifically, Li-ion concentration and potential profiles in the electrolyte phase were approximated by a polynomial function. A cubic polynomial was used for electrolyte concentration and potential inside electrodes, while separator liquid phase potential and electrolyte concentration were calculated by parabolas. Diffusion inside solid particles was simplified using an approximate solution based on the analytical solution for solid concentration. This type of reduced model could accurately predict the battery cell voltage with less than 1% error for discharging/charging current rates up to 5C, while the average computation time was reduced by a factor of 5.

2.1.4. Discretization-based method

For nonlinear PDE models, analytical solutions would become difficult to be derived. In this context, numerical methods could be employed to discretize the governing equations of PDE [94]. Finite-Element Method (FEM) is a numerical technique for discovering approximate solutions to PDEs. The FEM discretized the domain $x \in (0, L)$ into $N - 1$ subdomains. The Nth-order FEM approximation has N nodes. A FEM was used to develop three-dimensional thermal abuse model on lithium-ion batteries. A thermal model for a cylindrical battery was developed based on the FEM [34]. A particle-resolved 3D finite element model was implemented to study the effect of cathode microstructure on the electrochemical and mechanical responses of Li-ion batteries [95].

Finite Difference method (FDM) is the simplest and widely-utilized approach to handle the PDEs of battery electrochemical models. In the FDM, spatial domain is discretized into N nodes at $x = 0, h, \cdots, (N-1)h$, where $h = L/(N-1)$ is assumed constant for simplicity. Spatial derivatives are approximated by forward-difference, backward-difference, or central-difference. The mixed FDM was selected to discretize the spatial r, where the node points are unevenly spaced [30]. The mixed FDM can yield higher resolution with fewer node points in contrast to equally-spaced node points. The FDM was used to mesh the active particles along radial direction [32]. Then the complex PDE were discretized into ODEs and the state space expressiocn of system was obtained. The governing equations were discretized with central difference scheme for the first and second derivatives [96].

2.1.5. Physics-based equivalent circuit models

Due to the involvement of electric circuit elements to describe cell responses, ECMs can be identified rapidly. Here simplicity and practicability are two obvious merits for the application of ECMs [97]. However, ECMs also present the limited capability in terms of electrochemical mechanisms. Recently, P2D models have been simplified into the form of ECMs, which could significantly reduce the computational burden and enrich the physical meanings of ECMs. Finite volume method (FVM) was applied to a P2D model of Li-ion batteries [98]. The standard passive components were used to construct ECMs, indicating the energy storage nature of Li-ion battery. The parametric values of circuit elements were expressed as the functions of Li-ion concentrations and temperature. Results illustrated that the developed ECM could achieve close agreement with P2D model under a wide range of applied current rates, but occupies a much reduced computational resource. A novel implementation for P2D model was presented [99]. This model had a circuit-based structure without any simplification of the physical origins. A classic transmission line structure was used to replace the governing equations of current distribution within electrode. The concentration distributions were solved with the FDM. A new empirically parameterized physics-informed ECM was derived, as depicted in Fig.3 [100]. The P2D physics is discretized and represented as circuit elements in a network, requiring only 3 low-cost in-situ experiments: slow discharge, pulse discharge, and electrochemical impedance spectroscopy (EIS) under load. The model showed an accuracy of 19.6 mV compared to the multiple C-rate pulse loading experiments.

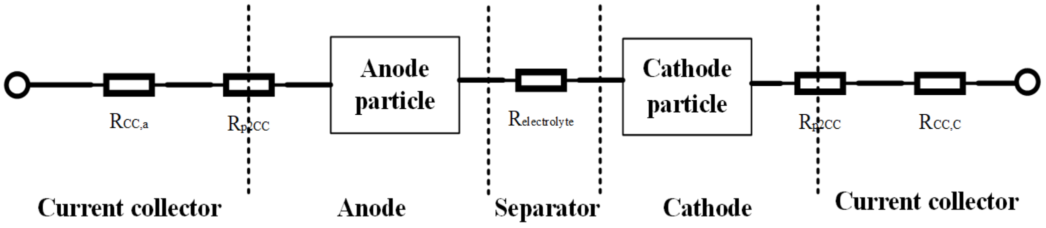

Figure 3: Cell level model schematic diagram for a single particle model [100].

2.1.6. Asymptotic reduction methods

Asymptotic techniques provide an effective means for model reduction and solution construction with clear ranges of validity. For example, the asymptotic reduction of P2D model was performed by Moyle et al. based on the fact that reaction kinetics dominate electrical effects [101]. They showed that the electric potentials are spatially homogeneous after asymptotic reduction and cell voltage behavior can be understood through a sequence of asymptotic regimes, which elucidates simple underlying physical processes.The asymptotic methods were used to reduce a thermo-electrochemical model and obtain solutions for common battery operation modes [102]. Asymptotic techniques were used to derive a thermal-electrochemical model systematically. The physical parameters and variables were nondimensionalized as:

$$\lambda = \frac{\Phi_0 F}{RT}, \delta = \lambda^{-1} \tag{15}$$

where R is the gas constant, T is the temperature, F is Faraday constant. All the variables could be expanded in powers of δ, using the notation as:

$$\begin{aligned} \Phi_k &= \Phi_{k0} + \delta \Phi_{k1} + o(\delta^2) \\ i_k &= i_{k0} + \delta i_{k1} + o(\delta^2) \end{aligned} \tag{16}$$

The leading order expansion was taken for model approximation. The reduced model was validated against a thermal P2D model and demonstrated very high accuracy with a computational cost reduced by over forty times [103].

2.2. Comparison and discussion

Table 2 summarizes various types of reduction methods for P2D model in terms of their reference, advantages and drawbacks. It should be known that the SPM based methods are the most widely utilized solution to simplify the P2D model. This method requires minimum computation resources and is able to provide sufficient model accuracy at low current rates. As an improved version of SPM, the SPM with electrolyte dynamics (SPMe) could predict the cell voltage at a high C-rate with lower computation burden than P2D model. However, due to the electrode width is much larger than particle radius, while only one particle for one electrode is insufficient, this SPMe would be limited for

Table 2: Different P2D model reduction techniques and their control-oriented applications.

Category	Simplification technique	Refs	Strengths	Weaknesses
SPM based	SPM	[80] [104] [105] [106]	Simple; Low computation burden;	Limited capability at high C-rates.
	SPMe (Improved with electrolytedynamics)	[107] [108] [79] [23] [109] [110]	Low computation burden; Enhanced performances at high C-rates, cell ageing, and thermal behavor; Easy for control-oriented implementations	Limited capability for cells with thick electrodes.
Transfer-function type	Residue grouping	[27] [111]	Low-order; Accurate in partial frequency range; Computation efficient;	Requiring pole/residue optimization; Prior-known parameters.
	Discrete-Time Realization Algorithm (DRA)	[28] [112]	Low-order; Accurate in overall frequency range; Computation efficient; Easy for control-oriented implementations	Prior-known parameters; Hard-to parameterize.
	Padé approximation	[89] [26] [29] [86]	Low-order; Accurate in partial frequency range; Computation efficient; Easy for control-oriented implementations.	Trade-off between order selection(accuracy) and computation burden.
	Integral method approximation (IMA)	[113] [31]	Low-order; Easy-to-derive; Computation efficient	Assumed Li-ion concentration profiles.

Polynomial expression	Parabolic functions	[93] [92] [114] [115]	Low-order; Easy-to-derive; Computation efficient;	Lacking physical meanings of polynomial coefficients.
Spatial Discretization	Finite-Element method (FEM)	[21] [35] [116] [34]	High accuracy	Heavy computation burden. Convergence requirement. Difficult for control-oriented implementations.
	Finite Difference method (FDM)	[96] [32] [117]	High accuracy	Sensitive to spaces and number of discretized nodes. Convergence requirement.
Physics-based ECMs	Physical analogies and interpretation	[98] [99] [33] [100]	Low-order; Easy-to-parameterize. Computation efficient;	Lumped parameters. Sensitive to the number of elementary sections;
Asymptotic reduction Leading-order approximation	Leading-order approximation	[103] [102] [101]	High accuracy; Computation efficient;	Nondimensionalized parameters; Labor-intensive model derivation; Hard for control-oriented implementations

Table 3: Different P2D model reduction techniques and their control-oriented applications.

Category	Cell state estimation	Optimal charge control	Fault diagnosis
SPM based	[24] [79] [118] [119] [120] [121] [122]	[123] [124] [125]	[126]
Transfer-function type	[127] [128] [129][130]	[131] [132] [133]	
Polynomial expression	[134] [135] [136]	[137] [76] [138]	[139]
Spatial Discretization	[140]	[141]	
Physics-based ECMs	[98] [142]	[143]	
Asymptotic reduction	None	None	None

cells with thick electrodes. For the transfer-function based solutions, although they are much more complicated than SPM based methods especially for transcendental transfer functions, this type of solutions could provide high accuracy in both frequency range and time domain. Specifically, residue grouping methods reduce the model order by optimizing the eigenvalues and residue vectors, while the residues would be grouped with similar eigenvalues. However, the electrochemical parameters must be given before residue grouping. DRA could also simplify P2D model to a low-order approximation and accurately match the frequency range. However, the battery electrochemical parameters must be known a priori, further making it difficult to parameterize DRA in an iteration process. The Padé approximation is an effective tool to convert transcendental transfer functions into polynomial expressions. The accuracy of the reduced model relies on the order selection of Padé approximant. A high-order approximation could provide sufficient accuracy at high frequency but at the cost of increased computational efficiency. Under the assumption of Li-ion concentration distributions, the integral approximation method is a much simplified approach to derive the transfer functions of reduced models.

For the polynomial expression-based solution, the polynomial expressions of battery electrochemical variables are capable of providing accurate prediction with significantly reduced computational effort. However, in general, the coefficients of parabolic functions are empirically fitted, hence lacking physical meanings.

Spatial discretization-based solutions belong to the commonly utilized numerical approaches for simplifying P2D models. Here the FEM discretizes the domain into multiple subdomains. Due to the way of approximating solutions with numerous basic elements, FEM becomes the most accurate one with a heavy computational burden. For the FDM, it can also simplify P2D model with high accuracy. However, the spaces and number of discretized nodes for all numerical methods must be carefully determined to ensure reasonable convergence.

The physics-based ECMs are essentially physical interpretation of electrochemical mechanisms. Similar to ECMs, this type of solutions can be implemented easily but also reflects the electrochemical process to some degree. For the physics-based ECM, its model parameters are reduced by lumping the parameters, while its performance highly relies on the selection of the number of elementary sections.

The asymptotic reduction simplifies the P2D model by using a leading-order approximation. Here the electrochemical reactions at different time scales are considered. All the known electrochemical parameters are nondimensionalized. The derivation of the asymptotic reduction is relatively complicated.

The electrochemical model could enhance the battery control performances on cell state estimation, fault diagnosis, and health-aware optimal charging. The physical model parameters reflect the inherent characteristics of the cell. For example, the volume fraction of active materials and maximum lithium-ion concentration determine the cell capacity. Thus, the cell degradation mechanisms including the loss of recyclable lithium ions and active materials can be identified by observing these parameters. Similarly, the cell fault can be diagnosed through the estimation of the variation of the physical parameters. In addition, the electrochemical model could provide cell internal states such as the lithium-ion concentrations in the electrolyte and solid phase, side reaction overpotential, and reaction flux across the electrodes. These electrochemical states are related to the cell ageing process. Hence, cell health-aware control could be realized by optimizing these electrochemical states. To sum up, the electrochemical model represents the cell interior dynamics. This could be helpful to achieve accurate cell state estimation, fault diagnosis, and efficient charging control.

To be specific, the SPM model has better controllability and observability than the P2D model [139]. An adaptive unscented Kalman filter based on SPM was proposed to estimate the SOC, lithium-ion concentrations, and potentials [24]. The estimated internal information is valuable to avoid lithium plating. All estimated states were verified to demonstrate fast convergence, robustness, and high accuracy even with a 20% initial SOC error. By assuming that the total amount of lithium in the cell is known, the dynamical properties of the SPMe observer, including the marginal stability, local invertibility, and conservation of lithium can be exploited [79].

Besides, the convergent estimates of solid and electrolyte phase concentrations on high C-rate cycles and transient electric vehicle charge/discharge cycles were also illustrated. For phase-transition materials during the battery's normal charge and discharge operation such as $LiFePO_4$, a novel boundary observer to estimate the concentration of lithium ions together with a moving boundary radius from the SPM via the backstepping method for PDEs was derived [118]. During the lithium ions intercalation and deintercalation, the stress generation contributes to the electrode particle fracture. A coupled SPM-mechanical stress model was used to design an adaptive observer for cell SOC, electrode particle stress, and solid-phase diffusivity. The internal stress and SOH-related parameters are predicted from real-time electric current and terminal voltage measurements [119]. A model from the pre-compute set of physics-based reduced-order components that span the expected dynamics of the cell over its lifetime was presented. Two significant ageing mechanisms were considered: solid-electrolyte interphase layer formation in the negative electrode and material dissolution in the positive electrode. An interacting multiple-model Kalman filter was used to select the pre-computed model for accurate estimations of cell internal electrochemical variables and output terminal voltage [127]. A composite $LiMn_2O_4 - LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ electrode battery model was used in dual-nonlinear observers to estimate the cell SOC and loss of cyclable lithium over time [129]. The surface and bulk lithium concentration of each material as well as the current split between each material were predicted. The reduced-order model was incorporated in a sigma-point Kalman filter to enable measurement feedback to improve voltage and internal-variable estimates. The system was implemented in a microcontroller and proved to be valid for BMSs [130]. An electrochemical model-based solution provided a basis for an output-injection observer to estimate the SOC over a wide range of operations, especially at high discharge rates [135].

Battery fast charging is one of the most effective techniques that affect the acceptance of EVs. Increasing the charging current could accelerate the side reaction rate and contribute to lithium plating. In order to minimize degradation rate and reduce charging time simultaneously, a charging method considering different limiting factors, including surface ion concentrations and side reaction rate, are crucial for cell health-aware charging protocol. Based on SPMe, the dynamic programming (DP) technique was employed to find the trade-off between charging duration, solid electrolyte interphase (SEI) growth, and lithium plating. The experimental results showed that the optimized fast charging strategy could reduce the capacity fade significantly compared with the widely used constant-current constant-voltage (CCCV) charging method without sacrificing battery health [123]. An optimal charging current at different SOCs was found using nonlinear model predictive control, which reduces side reaction rate and lithium plating rate. Pulse discharging current was added to promote the lithium stripping. With a comparable capacity fade, the proposed charging method was tested to reduce 39% of charging time compared with 1C CCCV charging method [125].

Similarly, the fast charging protocol considering side reaction rate and ion concentration was proved to reduce more than 40% in charging time compared with normal charging method but with less capacity and power fade [124]. To prevent the internal short circuit caused by lithium plating at the negative electrode, a fast charging control algorithm with two closed loops were presented. One loop was an anode over-potential observer, whereas the second loop includes a feedback structure that adjusted the current based on estimated status of lithium plating. The results showed that the cell can be fully charged within 52 min without lithium deposition [138]. The electrochemical model parameters have rich physical meanings and were considered as the referenced values for a healthy battery. However, the battery fault conditions such as ageing, overcharge/discharge cause significant variations of parameters from nominal values. An output error injection-based partial differential-algebraic equation observer was applied to produce voltage error signals. These imposed error values could be used to detect the ongoing fault conditions of the battery [126]. The fuzzy logic system was used to detect any variation in battery cell parameters and diagnose battery faults accurately in real-time [139].

Table 3 summarizes different P2D model-order reduction techniques and their control-oriented applications to cell state estimation, optimal control, and fault diagnostics. It can be noted that SPM based models are suitable for developing cell state estimation, optimal control strategy, and fault diagnosis algorithms. The spatial discretization method is the most accurate technique. Commercial software such as COMSOL uses the FEM to solve the PDEs and is often used as the benchmark for evaluating the simplified models [35]. However, FEM is difficult to be implemented for control-oriented applications. The polynomial profiles and physics-based ECMs could significantly reduce the computational complexity. The transfer-function type and asymptotic reduction models could achieve high accuracy as well. However, the computational complexity of the asymptotic reduction approach is relatively high, further limiting its applications in real battery control-oriented management.

3. Extension of P2D model

As discussed in Section 2, battery P2D model is mainly based on the porous electrode theory. The P2D model would simplify the modelling of complex electrode microstructure with the volume-average method at a macroscopic scale where the ion transport dynamics in the electrolyte and electronic conduction process in the solid phase are all captured, and a microscopic scale on which the ionic diffusion inside the electroactive particles is also considered. Due to the computational burden and accuracy, the P2D model is mainly adopted for battery electrode structure design. However, the P2D model has several issues when it is used for the development of battery simulation technologies: First, the particle size is assumed to be uniform in a P2D model, which does not accurately represent the electrode topology such as the actual size distribution of particles, the agglomerate structure of particle in the cathode. Second, the positive electrode is regarded as a single component without considering the blended cathode active materials. Third, the Bruggeman equation is used to model the effects of porous structure on the ionic transport and taken as constant, ignoring the microstructure variability. The Fick's diffusion law oversimplifies the intra-particle ionic transport. To address these aforementioned limitations, some attempts including the development of multi-particle model, multiple-scale model, coupled ageing and thermal model have been made and summarized in this section.

3.1. Multi-particle model

Many intercalation materials exhibit phase changes during battery charging/discharging process. Phase transitions strongly affect the lithium distribution inside particles and change the particle potentials. LFP is a typical cathode chemistry with phase change [30]. The coexistence of Li-poor and Li-rich phases should be accounted for and the boundaries between these two phases should be tracked, while the P2D model fails to analyze this phenomenon [144].A many-particle model was introduced where particles within a porous electrode are allowed to randomly exchange Li+ ions and electrons through the electrolyte and conductive matrix, respectively [145]. A general explanation of the occurrence of non-monotonic chemical-potential behavior in LFP electrodes was presented through two possible scenarios of new phase formation in a many-particle system, as shown in Fig. 4. At location A, all particles behave as a single phase. At location B, two alternative scenarios are available to the particle ensemble. The bottom path is that a single particle will hose a two-phase region, the top alternative is that the other particles will contribute lithium to the filling particle so that the relaxed result will be either fully lithiated or delithiated particles. At location C, particles can internally host phase boundaries, or the particles can either be lithiated or delithiated to the stable locations (B and D).

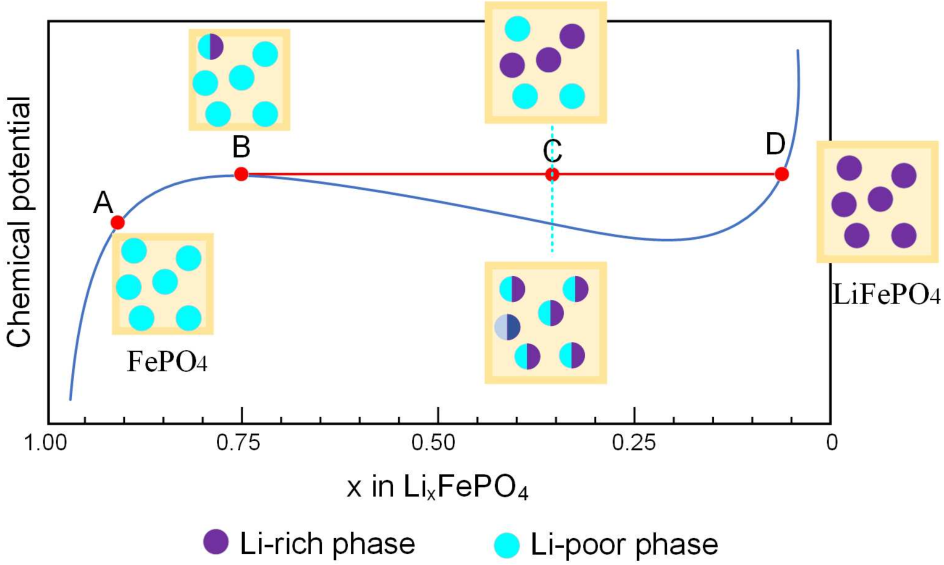

Figure 4: Chemical potential of LFP cathode evolution with two possible scenarios.

To develop an adequate modeling representation of the topology of the anode and cathode particles, Farkhondeh et al used a multi-particle model with variable solid-state diffusivity [146]. The memory effect of LFP electrodes was also analyzed. Simulation/experiment comparison for cells with the current rates up to 1C demonstrated the robust particle-size distribution estimation for galvanostatic charges/discharges. A 0D model of a phase separating active cathode particle based on multi-particle theory was derived. The dimensionality reduction is based on the volume averaging of dynamic equations [147]. The obtained 0D model has an explicit advantage of short computation time and high level of accuracy. A simplified physics-based model was derived combing the porous-electrode theory and multi-particles to predict a LFP-based electrode performance [48]. As shown in Fig. 5, four-particle bins were considered to represent the apparent particle size distribution (PSD) of the cathode. A polynomial approximation method was incorporated to model the effects of electrolyte. A fundamental analysis of the effect of particle size distribution on graphite electrodes and their performances was presented. The effects of particle heterogeneity on surface overpotentials were investigated [148]. It was concluded that for a graphite electrode, the surface-area- and volume-based approximations are sufficiently accurate for large- and small-scale PSDs.

The commercially available positive materials such as lithium ferrous phosphate (LFP), lithium cobalt oxides (LCO), lithium nickel manganese cobalt oxides (NMCs), lithium manganese spinel

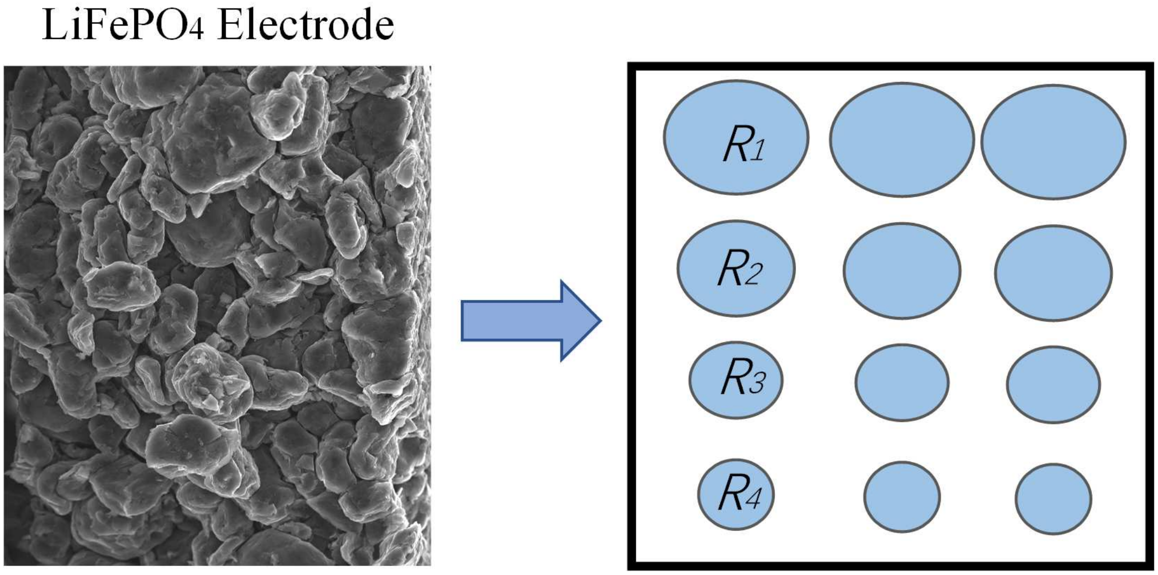

Figure 5: Schematic diagram of the LFP cathode that is assumed to contain four particle sizes

(LMO), and lithium nickel cobalt aluminium oxide (NCA), have their own characteristics in terms of power and energy costs. To obtain an acceptable trade-off between these characteristics, battery manufacturers would mix two or more positive materials to form a blend electrode. However, the P2D model assumes the single composition of the active material.A Li-ion mathematical model was developed to treat two positive-electrode materials ($Li_yNi_{0.80}Co_{0.15}Al_{0.05}O_2 and Li_yMn_2O_4$) [149]. To match the behavior of high rate discharge and impedance data, multiple types of electronic connections between particles and particle-conductive matrix were required. An extension of P2D model, accounting for the agglomerate of active material particles, $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NCM) and $LiNi_{1/3}Co_{1/3}Al_{1/3}O_2$(NCA), was derived by Leuth et al. [150]. The morphology of agglomerates can be seen in Fig. 6a. Micro-sized spherical secondary particles are the agglomerate of nanometer-sized primary particles which would be held together by binder [151] as shown in Fig. 6b. The model assumes that the liquid-transport is faster than the solid phase transport, while the electronic conductivity within agglomerate is sufficiently high. Therefore, the concentration polarization is significantly smaller than compact particles, which alleviates the rate-limiting effect of the solid diffusion on compact particles.

A $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2 - LiMn_2O_4$ (NMC-LMO) blended cathode obtained from a commercial Li-ion battery was considered [152]. As NMC forms agglomerates, it was divided into two classes of particles, i.e., primary particles and secondary particles. The secondary particles are assumed to be large non-porous NMC agglomerates. Three distributions from LMO particles, NMC primary particles, and NMC secondary particles were accounted for the multiple particle sizes of the active materials. The model could accurately capture the galvanostatic discharge at various current rates. The P2D model was modified to accommodate a composite electrode of $LiMn_2O_4$ (LMO) and $Li_{1/3}Ni_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC), as shown in Fig 6c [129]. A composite electrode is viewed as two parallel particles, one representing each active material. The negative electrode is a single material graphite electrode. The presented model structure was applied to battery SOC/SOH co-estimation. A high-power cell with lithium manganese spinel and lithium cobalt oxide at the positive while lithium titanate at the negative with 2 particle populations was studied with an SPMe model [153]. A simplified electrochemical model was developed to describe and maximize the specific capacity of battery cells through the variation of active (LFP)/inactive (carbon conductor and binder) ratios. The computation time was significantly reduced with these simplified models. Therefore, these reduced-order multi-particle models are

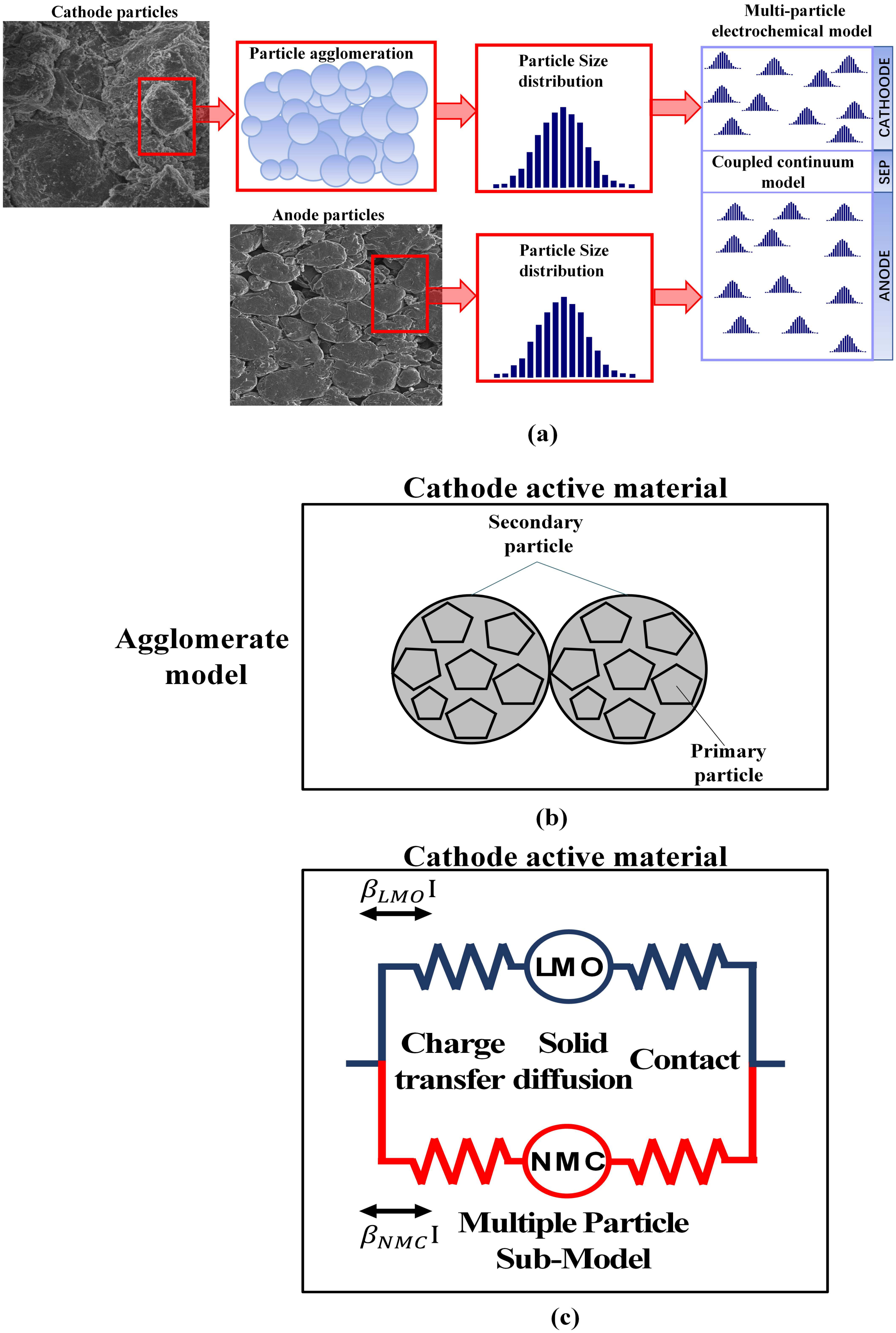

Figure 6: Multi-particle agglomerate coupling with P2D model(a), agglomerate model(b), and simplified multi-particle model(c).

promising for control-oriented applications [154].

3.2. Electrochemical model with multiple scales

The P2D model was derived by using volume averaging method (VAM), where the local microstructure features such as pore shape and localized current density distribution are neglected. This causes the P2D model become insufficient for applications involving active material utilization. The cell multiscale is depicted in Fig. 7. The macroscopic models from microscopic processes with one smaller length scale to account for geometric microstructure features such as pore shape was derived by mathematical homogenization theory derives.

The multi-scaled homogenized model is developed using asymptotic analysis of the microscopic model. The homogenization assumes that the porous electrode is composed of periodic micro-units. Each micro unit is composed of solid active materials S , electrolyte L, and solid-electrolyte interface T, as shown in Fig. 8. The ratio of micro unit length l to macro length L is denoted as spatial multiscale factor δ. $\delta = l/L$. Microdomain coordinate y and macrodomain coordinate x is converted by $y = x/\delta$. The basic idea of the homogenization method is to expand the system variables at multiple scales, and then substitute these expansions into microscopic equations to obtain PDEs with different scale components. Then, the expanded PDE is analyzed by δ at different orders [155]. The central ansatz for the expansions of the variables is:

$$
\begin{aligned}
c &= c_0(x,t) + \delta c_1(x,y,t) + \delta^2 c_2(x,y,t) + ..., \\
j &= j_0(x,t) + \delta j_1(x,y,t) + \delta^2 j_2(x,y,t) + ...,
\end{aligned}
\tag{17}
$$

So both the concentration and current density are dominated by the variations of battery length scale with relatively smaller variations on the electrode-particle length scale. The current density j flows around the electrode particles and hence displays significant variations on the particle scale.

A comparative analysis of the full homogenized model and P2D model was conducted [156]. The results illustrate that the predictability of P2D model deteriorates when predicting battery voltage response at low SOC for high operational temperature under 1C discharging case. The P2D model failed to capture the polarization of electrolyte under these scenarios, as shown in Fig. 9. Therefore, the homogenized macroscopic model presents a wider range of applications. A homogenized model was developed, which considers lithium diffusion within particles, lithium transfer from particles to the electrolyte and transport within the electrolyte. It was found that for low discharging currents, battery acts almost uniformly [157]. When the current is increased to a critical value, Li-ions in some regions of the battery are depleted, leading to the spatially nonuniform use of electrode. The conversion of homogenized equations to P2D model was carried out by Ciucci et al. [155]. The results indicated that the classical Doyle-Fuller-Newman (DFN) model is only the 0th order terms of the expansion. More specifically, the DFN-based approach is only valid under the assumption that $\delta \ll 1$. Ciucci's analysis was extended by computing the asymptotic order of interface exchange current densities, which is an important factor in the homogenization study [158]. As the commonly used Bruggeman's formula may in fact violate the physical bounds in some regimes, the exact values of the different effective transport coefficients were investigated [159]. An extended homogenized porous electrode model was presented considering the electrochemical coupling between particles of a real particle size distribution obtained from tomography data. The vanishing plateaus in the graphite potential curve with increasing charge or discharge rates was explained [160]. The P2D model is difficult to predict the heterogeneous reactions within the porous media with complex microstructures. An accurate standard homogenization of the battery was presented to analyze how the fluctuations occur and estimate them theoretically [161]. However, it should be noted that the control-oriented applications of the homogenized model are rarely-researched.

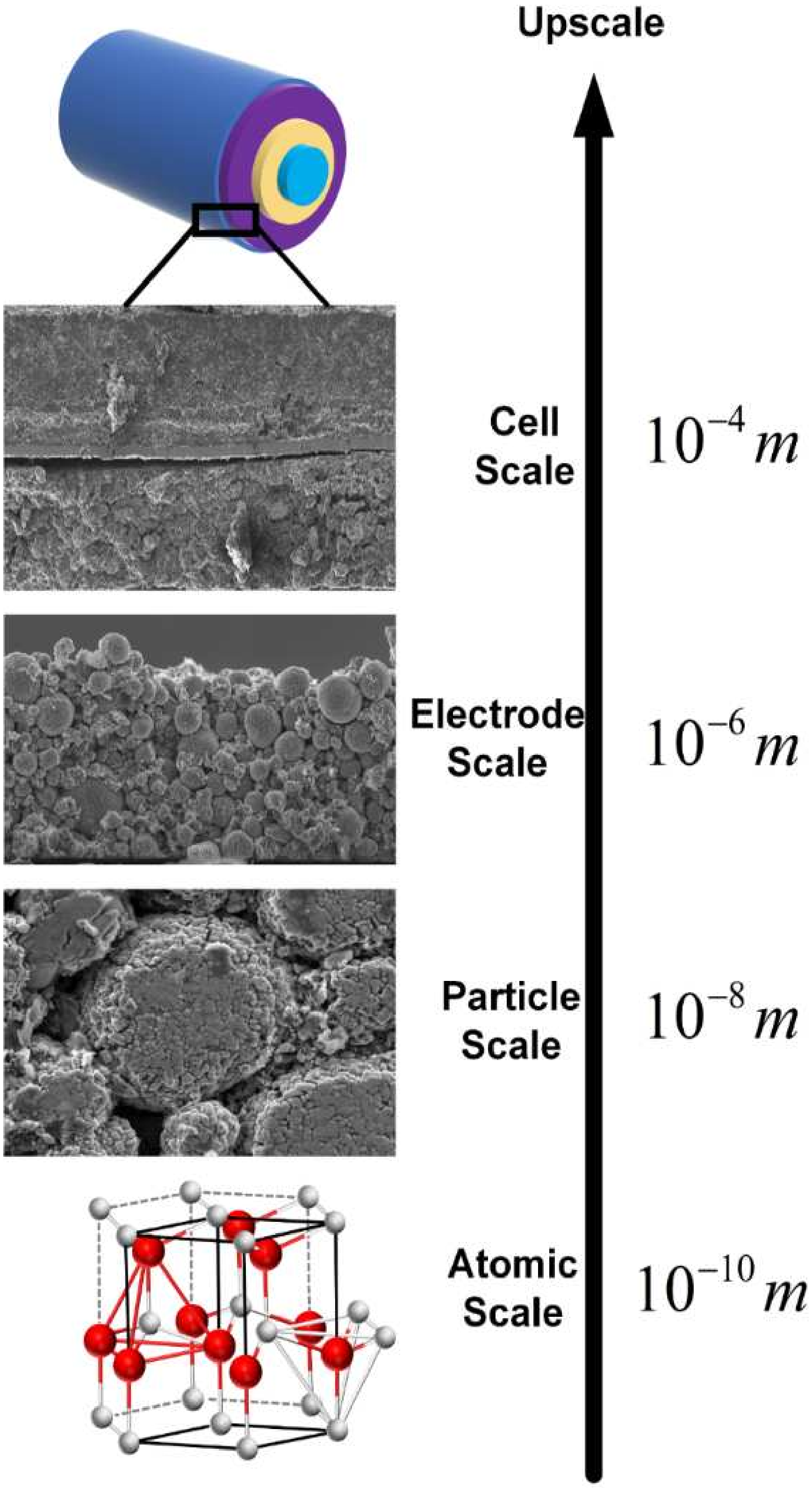

Figure 7: Li-ion battery structures at multiple length scales.

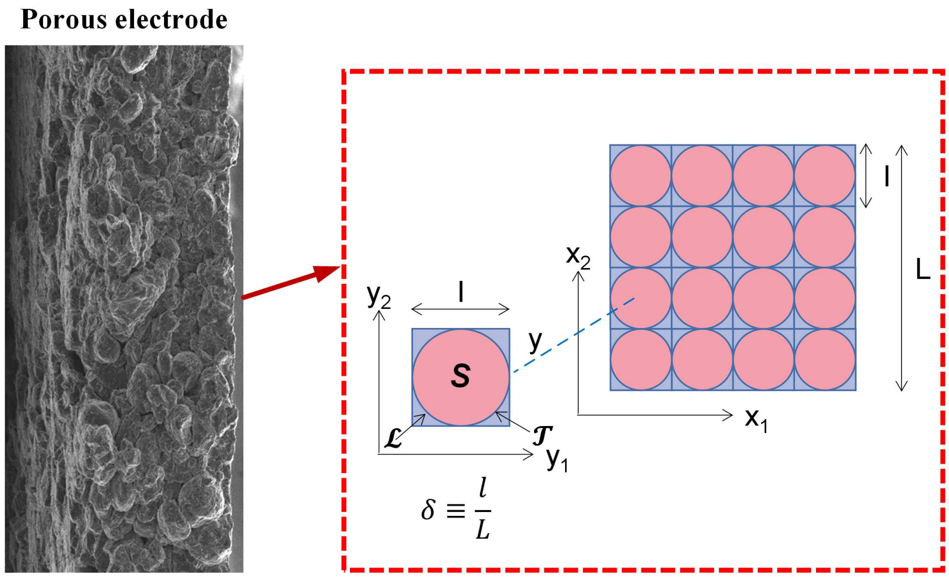

Figure 8: Representation of the porous electrode of a lithium-ion battery in the form of spatially periodical unit. Every unit cell **y** is composed of active particles **S** and electrolyte solution **L**, that are separately by an interface **T**.

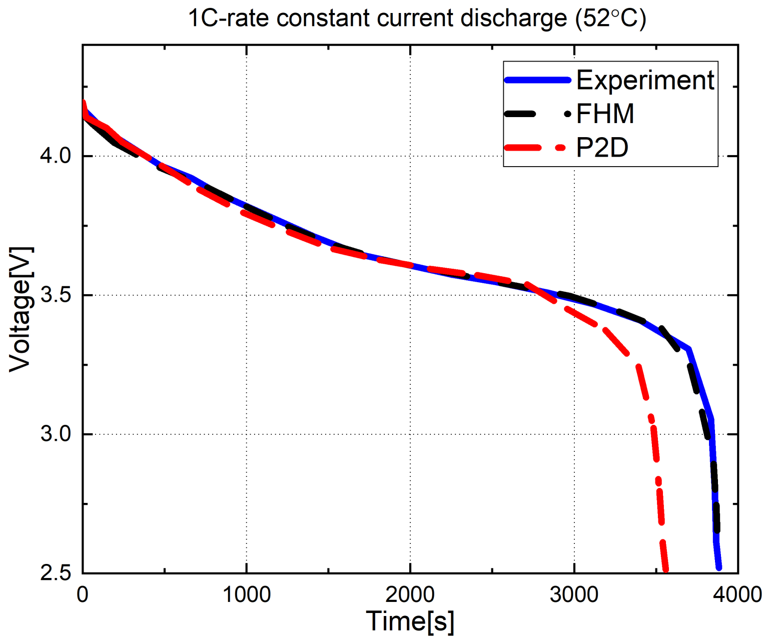

Figure 9: Performance of the P2D model and full homogenized model (FHM) against measured voltage from 1C-rate discharge test conducted at $52°C$ [156].

3.3. Electrochemical model with ageing and thermal effects

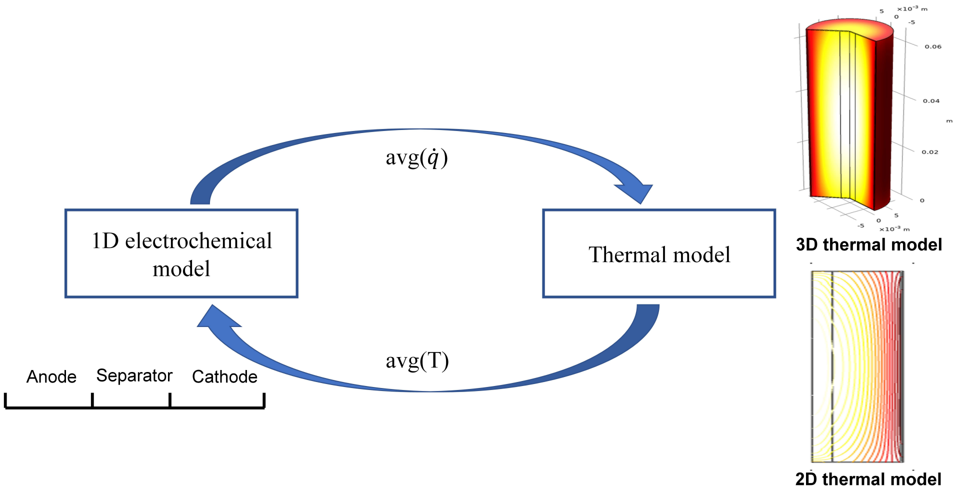

Figure 10: The coupled 1D electrochemical model and thermal model

Besides, apart from electrochemical behaviors, battery thermal and ageing (degradation) dynamics also plays a vital role in determining battery performance. In this context, battery electrochemical model is worth being expanded to consider these two aspects. To achieve this, one classical solution is to extend P2D or simplified 1D electrochemical models to 2D or 3D thermal models. In this way, two sub-models including an electrochemical model and a thermal model would be operated simultaneously. As illustrated in Fig. 10, a 1D electrochemical model would predict the heat generation rate (Qh) and voltage (V) of battery cell through various loading cycles. The voltage at a point from 1D model which corresponds to the tab of battery cell is then mapped to the tab of 2D thermal-electric model, and this battery 2D model allows the consideration of both temperature and current distributions across the surface of battery cell [162].A 1D electrochemical model was adopted to calculate the heat generation rate, as depicted in Fig. 10 [163]. Then the heat source is coupled into a 3D thermal model for calculating the temperature distribution inside a battery. The obtained average temperature would affect multiple parameters within the electrochemical model. As a result, the heat generation rate of 1D model would vary based on different temperature-dependent parameters. In the thermal model, the energy conversion equation based on the basic principle of heat transfer can be given as:

$$\rho C_p \frac{\partial T}{\partial t} = \lambda_x \frac{\partial^2 T}{\partial x^2} + \lambda_y \frac{\partial^2 T}{\partial y^2} + \lambda_z \frac{\partial^2 T}{\partial z^2} + \dot{q} \tag{18}$$

where λ_x, λ_y, and λ_z are thermal conductivities in the x, y, and z directions of the battery, respectively. The value of $\dot{q}$ refers to heat generation in the cell, which includes reversible heat and irreversible heat. The reversible heat is mainly related to the entropy change of the electrode active material. The irreversible heat consists of the active polarization heat arising from the electrochemical reaction and ohmic heat.

Due to the increased complexity of coupled multiscale model, the underlying physical models need to be simplified for battery control-oriented applications. [164] reported a reduced-order electrochemical thermal model of a pouch cell. The ion concentration within an electrode is approximated using the polynomial approach, while the ion concentration within electrolyte is simplified using the state space method. Both potentials and electrochemical kinetics are linearized. Cell temperature is calculated based on the energy conversion formula to further determine the temperature-dependent diffusion coefficients. Then the model performance is evaluated by analyzing appropriate experimental data at multiple cycles under different operational conditions. Illustrative results confirm that the computational effort of the reduced-order model (ROM) would be reduced to the fifteenth, while its accuracy can be still maintained. It should be known that various simplified versions of coupled models have been proposed. For example,the accurate electrochemical and thermal response of Li-ion cells were explored [165]. Here the local heat generation and spatial temperature variation are volume averaged to derive the reduced-order coupled PDEs of battery electrochemical-thermal model. This ROM structure could be easily utilized for parameter identification of controlling processes at high current rates. A control-oriented thermal-electrochemical model was developed and well validated for the commercial prismatic battery [166].Here the multilayer thermal model and polynomial approximation method are applied to describe battery thermal behavior and electrochemical process, respectively. This 3D battery model is divided into dozens of thermal nodes connecting by the thermal resistances. The multiplayer thermal model is constructed by using thermal balance equations for all thermal nodes.

In addition, the coupled electrochemical-thermal model also allows the investigation of ageing effects concurrently. It should be known that battery ageing significantly depends on temperature and could lead to significant heat release. Ageing would generally occur at the active material particle scale, while heat transport occurs at the cell scale. Kupper et al investigated the battery multiscale heat, mass transport and complex electrochemical reaction mechanisms based on a coupled model [167]. Here this coupled model is derived by considering the homogenization of three 1D models: one for intra-particle lithium diffusion, one for electrode-pair mass and charge transport, and one for cell-level heat transport. The main and side reactions are described with the flexible multi-phase electrochemistry. Besides, the thermal model is able to provide a feedback between temperature and battery electric dynamics as well as ageing. One of the challenges for anode side is that dendritic and mossy lithium surface can form solid electrolyte interphase (SEI) easily during cycling, as shown in Fig. 11 [168]. For fresh anode surface, the particles are covered with an SEI layer. When the anode is lithiated during charge process, a large volume expansion occurs as shown in Fig. 11B.The SEI layer could be damaged, leading to the exposure of the particles to electrolyte.Hence, a thicker SEI layer would form consuming the lithium inventory as depicted in Fig. 11C. After many cycles, a much thickened SEI evolves as shown in Fig. 11D. For the cathode side, higher mechanical stress would accelerate the cracks and de-cohesion of particles. Furthermore, the cathode-induced oxidation of solvents will cause gas generation [95].

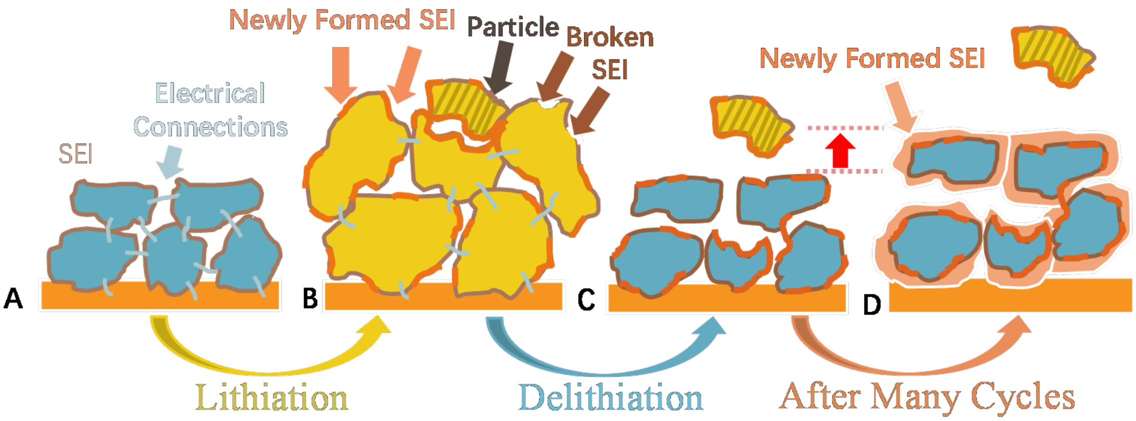

Figure 11: Scheme of negative electrode degradation mechanisms [168].

A simplified electrochemical and thermal ageing model [169] was presented. Here the mechanism of porosity modification caused by the growth of solid electrolyte interphase (SEI) film at the negative electrode is incorporated into the electrochemical and thermal models. Illustrative results indicate that the cracking and fracture of SEI layer would be significantly affected by cycling operating conditions and play an important role in accelerating the electrochemical mechanisms.A growth rate of around 0.64 nm/hr at 1C for the SEI film on the negative electrode was observed. In addition, for a convective heat transfer coefficient (h) larger than $1W/(m^2K)$, there is limited effects of battery ageing model on surface cell temperature [170].

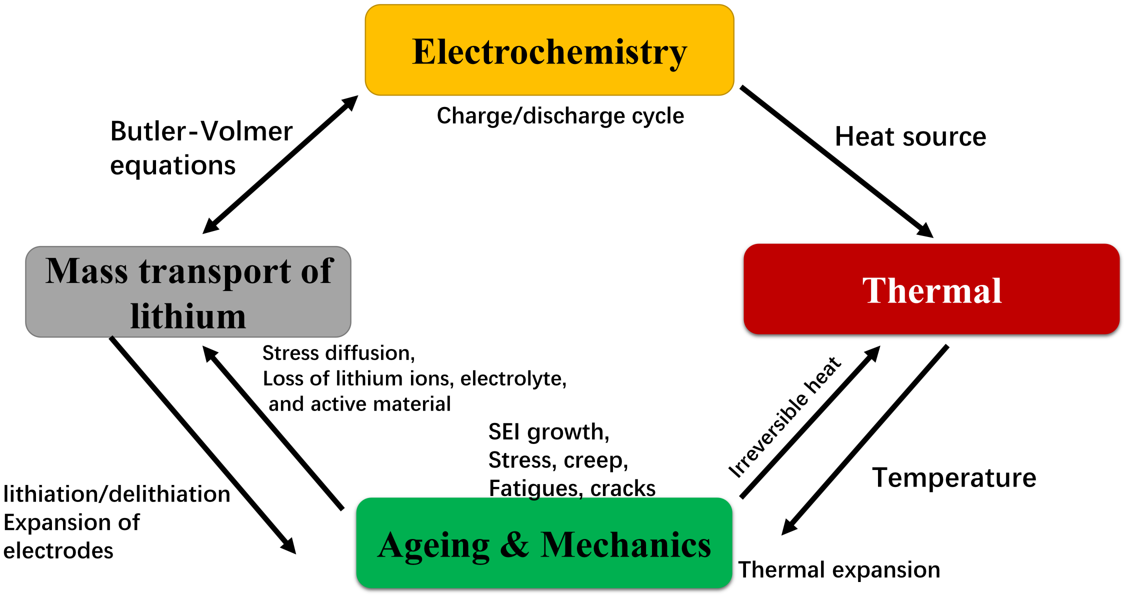

Figure 12: Main coupling phenomena.

In theory, mechanical strain would also play a pivotal role in affecting battery durability. In this context, the coupling between battery electrochemical and mechanical dynamics can also provide significant insights into cell degradation. The thermo-mechanical behavior within a multilayer section of lithium 18650 cell during discharge [171] was evaluated.

The equation of heat transfer in each part of the cell is expressed by:

$$\frac{d}{dt}(\rho C_p T) = -div(-\lambda grad(T)) + \dot{q} \tag{19}$$

where T denotes temperature, ρ density, C_p specific heat capacity, λ thermal conductivity and $\dot{q}$ heat sources.

The heat generation $\dot{q}$ per unit volume of the cell is given as:

$$\dot{q} = \frac{1}{V_{bat}}[i(V - E_{OCV}) + i(T\frac{dE_{OCV}}{d_T})] \tag{20}$$

where i is cell current,V is battery potential, E_{OCV} is open-circuit voltage and V_{batt} is battery volume. The partition of strains leads to write the total strain as the sum of all possible strains:

$$\varepsilon_{total} = \varepsilon_e + \varepsilon_T + \varepsilon_L \tag{21}$$

where ε_e is the elastic strain tensor, ε_T is the thermal strain tensor and ε_L is the lithiation/delithiation expansion of electrodes. The stress-strain relationship is:

$$\varepsilon_e = \frac{E}{1+\upsilon}\sigma - \frac{\upsilon}{E}tr(\sigma)I \tag{22}$$

E is the Young's Modulus, v is the Poisson ratio and I is the identity tensor. The thermal strain is expressed by:

$$\varepsilon_T = \alpha(T - T_0) \tag{23}$$

where α is the coefficient of thermal expansion, T_0 is the initial temperature and T is the actual temperature.

As shown in Fig. 12, lithium diffuses in the lattice of electrode structure at the electrode scale, further leading to structural changes and mechanical stresses. At the same time, the macroscopic electrochemical model calculates the heat generation caused by the ohmic losses, charge transfer overpotentials at the interface, and mass transport limitations. These factors contribute to the mechanical stresses.It is illustrated that the gradients of lithium concentration determine the stress level, and large stresses are generated at the electrode-separator interface when high current rates are applied [172]. A coupled electrochemical-thermal-mechanical model was used to investigate Li-ion battery degradation. It was found that high temperature can accelerate battery SEI growth, while low temperature would cause severe lithium-plating. Current with high rates would increase the diffusion-induced stress significantly and result in severe cathode active material loss [173]. These reduced electrochemical-thermal models could benefit the accurate cell state estimation and optimal charge control, especially for all-climate electric vehicles.

3.4. Discussion

This section summarizes the extended variants of the P2D model, including the multi-particle models, multi-scale models, ageing, and thermal models. These models make up for the deficiency of the P2D model. Specifically, the multi-particle models are suitable for cathode materials with significant phase-transition such as LFP, where the particle interactions dominate the electrode performance. The inhomogeneity of the particle distributions can be captured by the multi-particle models. Thus, they are appropriate for composite electrodes, where two or three types of active materials are mixed, and electrodes composed of agglomerated particles. The multi-scale models are of great interest when the electrode microstructures are concerned. They are derived with asymptotic methods and could outperform P2D model at low SOCs and high temperatures. The ageing and thermal effects are critical aspects of long-time battery modeling [174]. In general, the ageing and thermal effects are coupled with the electrochemistry phenomenon. The combined electrochemical-ageing-thermal models are powerful tools to depict the multi-physics cells. In summary, these extended electrochemical models are promising for achieving effective performance under control-oriented applications where the typical P2D model fails.

4. P2D model parameterization

Parameter identification of electrochemical model is also important for accurate model-based battery state estimation and optimal control design. As the PDEs within P2D model contain many physical parameters, it is a key but challenging task to identify all these parameters. First, battery manufacturers generally do not disclose this information in their manufactured battery specification sheet. Second, the measurable signals including voltage, current, and temperature present the complicated nonlinear relations with these parameters. The parameter identifiability would vary for different operating conditions, further complicating the parameterization goal. Third, various characterization and expensive instruments are required to measure these parameters. Furthermore, the parameters are specific to each cell design (including geometry and chemistry), leading to the fact that not all parameters could be transferable from one cell design to another. One common-utilized approach is to fit the parameters of electrochemical model for matching the measured cell terminal voltage, which is sensitive to the initial set of these parameters [175]. In many related research, these parameter sets are generally adopted from literatures, while their origins are seldom traced. Another typical solution is to measure these parameters experimentally. In this section, two widely adopted methods, including direct measurements and noninvasive parameter estimation, are summarized and discussed.

4.1. Physical parameter measurements

For the physical parameter measurements, parameters of battery electrochemical model would be obtained directly through cell post-mortem analysis [176]. For example,a physio-chemical model was fully parameterized for a high-energy pouch battery cell [177]. Specifically, battery cell was opened under argon atmosphere for the measurements of geometrical data. The porosity, particle radius, and tortuosity of the electrodes and the separator were determined with Hg-porosimetry. Electrolyte conductivity and diffusion constants, as well as electronic conductivity were detected by using the voltage response to a dc current. The electrode open circuit voltage curves, diffusion coefficient, and charge transfer kinetics, were measured on the reconstructed coin cells. The parameterized physico-electrochemical model was validated against the commercial cells with same chemistry [178]. Johannes extracted the physical parameters from a high-power prismatic cell. The composition as well as the porous structure were measured using optical emission spectroscopy and Hg-porosimetry. The electrochemical properties of electrode materials were determined using coin cells with lithium as counter electrode [179]. Relative validation showed that the behavior of full cell can be reproduced from the parameterization of individual material parameters with small errors [180]. The experimental methodologies for cell teardown and subsequent chemical, physical, electrochemical kinetics, and thermodynamic analysis was presented. The cell consists of a NMC positive electrode and graphite-SiOx negative electrode. The electrode open-circuit-voltages (OCVs) and lithium stoichiometry were obtained using galvanostatic intermittent titration technique(GITT) in half cells. The electrochemical impedance spectroscopy (EIS) measurements were used to determine the activation energy and exchange current coefficient [181].

Table 4 summarizes several physical parameters of electrochemical model and their related measurements. The geometric configuration of a cell, as well as the domain morphologies within the cell, are determined by manufacturing processes. The electrode plating area, current collector/electrode/separator thickness are straightforward to be understood and are relatively easy to be measured through using calipers or a micrometer gauge. Scanning electron microscopy (SEM) is an effective tool for 2D image acquisition. These obtained 2D images can be then processed to extract measurements for layer thickness, particle radius, and particle size distributions [179]. SEM was combined with FIB to investigate the 3D microstructure of electrode, while the porosity was calculated based on these images [181]. The tortuosity can also be calculated from these images. Mercury porosimetry is a destructive technique to measure porosity, pore volume, and pore size distribution. The mercury is forced into small void spaces in the porous medium, and the volume of intruded mercury was recorded [177]. GITT is a method that can measure the open circuit potential and solid-phase diffusion coefficients [193]. The activation energy and exchange current density can be determined by using EIS [178]. In terms of the chemical properties, elemental composition of the active materials can be analyzed by using energy-dispersive X-ray spectroscopy (EDS) and inductively coupled plasma optical emission spectroscopy (ICP-OES).

4.2. Noninvasive parameter estimation

On the other hand, noninvasive parameter identification methods have been investigated widely without the need of tearing down battery cells, where related parameters are estimated by fitting the model responses to the experimentally measured voltage [194]. Parameter identifiability belongs to a model basic property to describe whether the parameters of model can be identified from its output for a specific input. In general, parameters with high sensitivity could be identified accurately with

Table 4: Physical parameters and their characterization method.

Physical parameters		Characterization method
Geometrical	Electrode plating area	Disassembly and direct measurements [181, 177, 180]
	Current collector thickness	Disassembly and direct measurements [181]; ICP spectrocopy [177];SEM images [179]
	Electrode/separator thickness	Disassembly and direct measurements [181, 177]; SEM images [180]
	Particle radius	SEM images [181];Hg-porosimetry [177, 180]
	Porosity	SEM-FIB [181]; Mercury porosimetry [177, 180]; liquid absorption [182]; X-ray micro CT [183]
	Tortuosity	SEM-FIB [181]; Hg-porosimetry [177, 179]
Electrochemical	Solid-phase lithium diffusivity	GITT [181] [179] [184] [99, 185];EIS [177]; CV[186]; PITT[187]
	Solid-phase electronic conductivity	Four-point probe [181]
	electrolyte electronic conductivity	EIS [188]
	Open circuit potential	GITT [181, 144]; Slow charge and discharge [180] [189][190]; Three-electrode method [181]
	Activation energy	EIS [181];GITT& EIS [177];GITT [179];
	Reaction rate constant	EIS [181, 177];CV [191, 192];
Chemical	Active material composition	EDS [181];ICP-OES[179]
	Electrolyte composition	Gas chromatography [179]; Ion chromatography [42]

designed experiments [195]. For instance, an effective way through combining parameter analysis and identification to determine a battery electrochemical model [196] was presented. Here the Fisher-information matrix approach in combination with a sensitivity analysis was derived to estimate the identifiability of each parameter. Then the number of experiments would be reduced to a relatively small one, while 33 electrochemical parameters could be fully parameterized based on this sensitivity information.The full set of P2D model parameters were identified from cycling data based on a genetic algorithm, where the accuracy and identfiability of the resulting full parameter set were assessed using Fisher information [197]. The most identifiable condition for each parameter was proposed based on the sensitivity analysis and clustering analysis. Then the highly sensitive parameters were identified under such condition [57]. Some researchers determined the specific subsets of parameters rather than identifying all the parameters, while other parameters were taken from the literature [88].

The adopted optimization algorithms, number of estimated parameters, optimization objectives, and experiments for estimating parameters of battery electrochemical model are summarized in Table 5. As shown in Table 5, the number of estimated parameters would vary significantly on different publications. This difference is mainly caused by the model complexity, estimation procedure, and optimization objective (e.g., whether temperatures and EIS-based frequency responses are modeled). Here the most commonly used optimization algorithm is the gradient-based algorithm, such as the least-square algorithm [196], Levenberg-Marquardt algorithm [199], and Genetic algorithm [88]. Recently, the neural network based algorithms have been also used to estimate the parameters of electrochemical model. For example, a deep Bayesian neural network was used to identify optimal parameters [202]. Results illustrated that the neural network based method require less calculation time than genetic algorithm, particle swarm optimization, and Levenberg-Marquardt algorithm. Apart from time-domain signals of battery such as terminal voltage and temperature, the frequency test via EIS was incorporated in the parameterization [203]. The identification process was divided into four tests and eight steps, where the number of parameters to be identified in each step is significantly reduced [203].

4.3. Discussion

This section summarizes two practical model parameterization methods: direct parameter measurements and noninvasive parameter identification. Each method has its strengths and weaknesses. The direct parameter measurements could provide the exact parameter values through post-mortem analysis, which is robust and accurate. However, this process is costly and time-consuming, since the cell teardown and subsequent chemical, physical, electrochemical kinetics and thermodynamic analysis should be carefully conducted. The specific instruments for conducting these studies are expensive. For noninvasive parameter estimation, this method is highly dependent on the identifiability and sensitivity of these parameters. The quality of training data and preset parameter variation range are critical to achieving ideal results. This method indeed could save much parameterization efforts if these requirements are met. The parameter identification results determine the efficiency of the electrochemical-model-based applications. Therefore, the researchers should pay attention to the detailed parameter identification method and select the appropriate protocols.

5. Challenges and Perspectives

In this section, the challenges for tackling the limitations of classical battery P2D model, incapability of model-order reduction techniques, and bottlenecks of model parameter identification are discussed. Then some perspectives to further handle these issues towards battery electrochemical model-based control-oriented management are given.

Table 5: Parameter estimation algorithm, number of estimated parameters, used optimization objectives, and required experiments for model identification.

References	Optimization algorithm	Number of estimated parameters	Optimized objectives	Experiment
[196]	Least-square	33	Voltage Temperature	C-rate and pulse tests
[197]	Genetic algorithm	88	Voltage	Drive cycles
[198]	Tuned	41	Voltage Temperature	C-rate tests
[199]	Levenberg-Marquardt algorithm	21	Voltage	C-rate and pulse tests
[200]	Particle swarm optimization	4	Voltage	C-rate and pulse tests
[201]	Evolutionary algorithm	11	Voltage	C-rate tests
[56]	Least-square	7	Voltage	Pulse tests
[69]	Hybrid optimization algorithm	44	Voltage	C-rate and pulse tests
[202]	Deep Bayesian neural network	6	Voltage	C-rate and pulse tests
[203]	Particle swarm optimization	14	Voltage, EIS data	C-rate and pulse tests, EIS test.
[204]	Generalized reduced gradient optimization	20	Voltage	Linear-sweep voltammetry
[205]	Cuckoo search algorithm network	26	Voltage	C-rate and drive cycles
[206]	Particle swarm optimization	28	Voltage	Pulse test

5.1. Challenges

Limitations of P2D model: Battery electrochemical model presents great promise for understanding the fundamental mechanisms of existing battery materials and components, while the dynamics and performance of new battery materials and components could be also predicted. The P2D-based battery modeling framework has become an ubiquitous tool to perform cell-scale simulations of Li-ion batteries. This accelerates the wide deployments of electrochemical model-based control algorithms for onboard battery state estimation, optimal charge/discharge control, and fault diagnostics. Despite the widespread usage of battery electrochemical model, its challenges towards control-oriented battery management still remain. P2D model ignores the details of electrode microstructure and describes them as homogeneous media in which electrolyte and solid materials coexist at each point. This assumption is invalid when it is necessary to capture local microscopic effects, especially the interaction between microstructure, degradation, and heat. Thus, macroscopic P2D model cannot fully depict the cell dynamics at extreme operating conditions, such as low SOCs and low temperatures. Furthermore, P2D model employs Fick's law to determine the lithium diffusion in active materials. For phase-change materials, such as LFP, the P2D model fails to provide accurate predictions on intra-particle diffusions. Fast charging remains the bottleneck technique to increase the willingness of consumers to purchase EVs. The physical model-based optimal charge protocol is promising to accelerate charging speed and alleviate cell degradation [125]. However, most of the published works on battery electrochemical modeling were validated to achieve accurate predictions with constant discharge scenarios [93]. The evaluation of model performance with charging condition, especially at high C-rates is rarely-seen and worth exploring.

The incapability of model-order reduction techniques: The rigorous P2D model should be properly simplified and tailored for control-oriented applications. SPM based algorithms are among the most practical applications [207]. In general, ROMs are linearized around preset equilibrium points. For example, the Bulter-Volmer equation was linearized around a set-point that includes zero reaction flux (i.e.,$j_0 = 0$) (16). However, as the input current and reaction flux increase, ROM derived from $j_0 = 0$ would become no longer accurate. In this context, model performance far from equilibrium conditions need further investigation. Prior knowledge of battery characteristics, including battery chemistry, rate capability, and parameter sets of electrochemical models, is necessary to develop ROMs. Each model order reduction technique has its strengths and weaknesses. It is an ultimate goal of control-oriented model simplification to reduce the computational burden while maintaining the predictability of integrated model. Unfortunately, no such a simplified model could meet all requirements to our best knowledge. Alleviating the computational burden while maintaining the comprehensive model predictability is an ultimate goal for control-oriented model simplification, where none such simplified model could solve all current issues.

Model parameter identification bottlenecks: The parameter identification of battery electrochemical model lays the foundation for the development of model-based control algorithms. However, as some parameters are difficult to be obtained through battery disassembly analysis, it becomes challenging to obtain a suitable set of parameters for battery electrochemical model. Currently, many parameters are still difficult to be fully identified from direct current and voltage measurements [208]. On the other hand, when using computational methods to estimate the model parameters, there are always some redundant parameters that cannot be identified directly. In this context, the lumped parameter reformulated models that minimize the set of parameters to be estimated by normalizing the geometric coordinates and grouping parameters that always appear together on the PDEs are recommended [209].

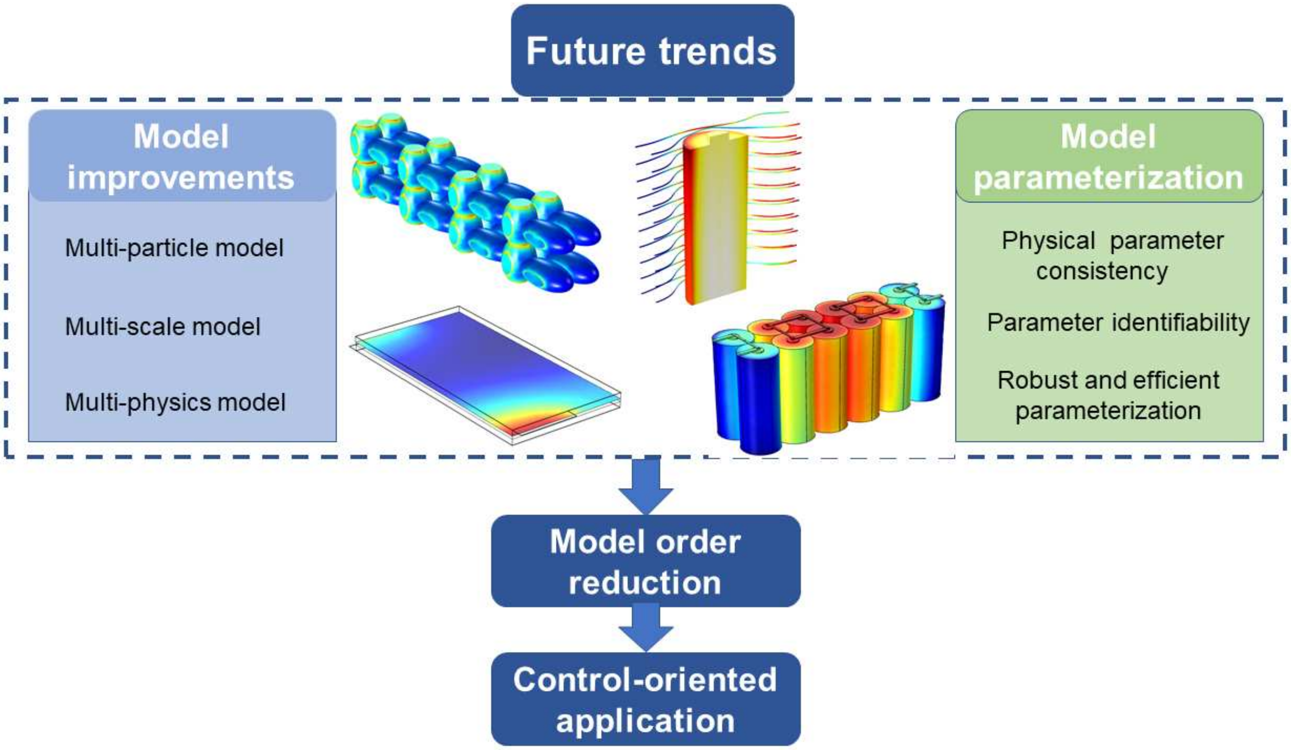

Figure 13: Future trends of control-oriented modeling.

5.2. Perspectives

The existing research rarely brings significant improvements on the aforementioned aspects. To further improve the performance of battery control-oriented electrochemical model so as to promote the development of next-generation BMS, the following aspects are suggested to be considered in future research, as illustrated in Fig. 13.

Model extension and improvements: For cases of great practical interest, such as LFP active material in Li-ion batteries, due to the interactions of multiple particles, the charge-discharge mechanism inside active particles has not been fully understood. Besides, typical P2D model cannot describe the microstructure of battery electrode, while the relevant developed microscopic model solution is still computationally more demanding than the P2D model. In this context, a reduced-order 3D microscopic model is urgently required. The ageing effects such as lithium plating are distributed within an inhomogeneous electrode structure. Lithium electroplating would cause the growth of lithium dendrites, which presents the risk of causing thermal runaway. This demands the development of coupled electrochemical models allowing the combination of local temperature, concentration fluctuations, and ageing processes. Similarly, the coupling of stress development from both the particle and electrode levels needs to be considered. For battery pack applications, the inevitable cell inconsistencies would lead to electrical imbalances. In this context, deriving efficient pack-level electrochemical model considering cell inconsistency becomes necessary.

Model parameterization: Model parameterization is still a bottleneck for wider applications of battery electrochemical model in control-oriented battery management. The consistency of assumptions for many parameters is still unclear. For example, numerous assumptions are typically made to parameterize a model (e.g., whether insertion materials are treated as spherical or planar for solid-state diffusivity inferred by EIS). Identifiability issue further complicates this parameterization challenge. In this context, more robust and efficient parameter identification methods are required [210].

6. Conclusions

With the rapid development of battery electrochemical models, the advanced electrochemical model-based BMS could achieve safe, efficient, and reliable control strategies for onboard Li-ion batteries. As a classical type of electrochemical models, the P2D model is difficult to be adopted directly for control-oriented applications such as cell state estimation, charging control, and fault diagnostics. Model simplification is thus crucial for converting P2D model governed by numerous PDEs to low-order linear models for real control applications. In this review, different P2D model-order reduction methods are first surveyed, where their advantages and shortcomings are discussed and compared. The survey has shown that the SPM-based protocols are the most popular approach for P2D model simplification. After analyzing the limitations of P2D model, enhanced solutions including the multi-particle model, multi-scale model, model with thermal and ageing elements are reviewed. Then the corresponding reduced versions of these enhanced electrochemical models are summarized as well to further benefit battery control-oriented management. As accurate model parameterization is also the key to the effective operation and control of Li-ion batteries, model parameterization methods including the direct parameter measurements and invasive parameter estimation are also summarized and compared. Based on these discussions, challenges, and perspectives on the development of control-oriented electrochemical models are finally presented.

In a nutshell, reliable control-oriented management of battery electrochemical model requires to be implemented for online application, but many corresponding technologies are immature. None of the electrochemical modeling solution is a one-size-fits-all strategy; instead there should be an inherent trade-off between the model complexity and performance. This review would provide useful reference points to support the design and operation of battery electrochemical model and parameterization, whilst also informing the agenda of the battery and control engineering communities.

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