



A non-iterative method for single particle models of lithium-ion batteries with electrolyte dynamics

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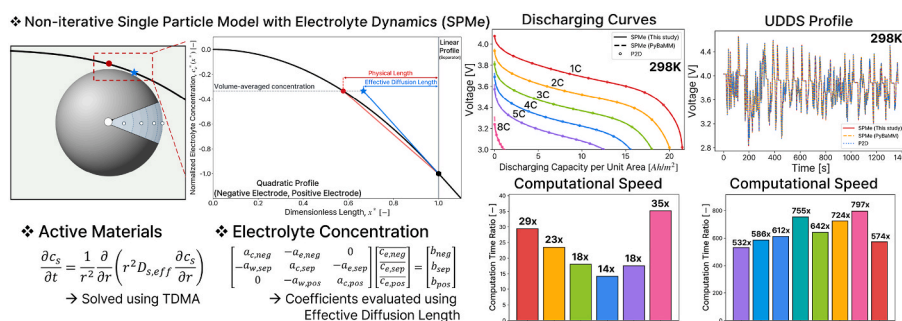
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HIGHLIGHTS

- A non-iterative method to solve SPMe is proposed.
- Effective diffusion length approach for transport in electrolyte is introduced.
- Voltage RMSE stays within ~ 5 mV against the P2D model at 273 K and above.
- The proposed method completes $\sim 10,000$ discharging simulations in 1 s.
- The proposed method serves as a foundation for simulation-intensive applications.

GRAPHICAL ABSTRACT



ABSTRACT

A non-iterative approach for solving the single particle model of lithium-ion batteries with electrolyte dynamics (SPMe) is proposed by strategically designing the solution procedure. First, solid-phase diffusion in the active materials is solved using the tri-diagonal matrix algorithm (TDMA). Next, by utilizing an effective diffusion length under uniform current density, the ion transport in the electrolyte is reduced to solving a 3×3 matrix. Then, with the negative electrode potential set to 0 V, and the negative electrode overpotential and the electrolyte potentials at both electrodes are evaluated analytically. Finally, the positive electrode overpotential and the equilibrium potential are added to the positive electrode electrolyte potential to determine the cell voltage. Through this process, the SPMe is solved non-iteratively while retaining concentration- and temperature-dependent electrolyte transport properties. As a result, a full constant-current discharge is solved in ~ 0.1 ms and a driving profile in 1 to 2 ms, enabling near-instantaneous simulation of battery behavior. Comparisons with the PyBaMM SPMe and the P2D model show that the present method reaches comparable voltage accuracy to the PyBaMM SPMe across various operating conditions. This method enables applications that require rapid, large-scale simulations, such as parameter identification and hardware-in-the-loop simulations.

1. Introduction

Lithium-ion batteries (LIBs) are the key element of modern energy systems, due to the substantial growth of electric vehicles (EVs) and

energy storage systems (ESS) [1–3]. Predicting battery behavior is crucial to monitor safety and extend lifetime in these large-scale applications [4–6]. While Equivalent Circuit Models (ECMs) offer computational efficiency for real-time simulations of key variables (e.g., voltage,

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temperature, current), they do not account for internal electrochemical states, leading to limited safety assessments [7–12]. In contrast, physics-based electrochemical models capture these internal behaviors, offering a distinct advantage over empirical approaches [13–16]. The Pseudo Two-Dimensional (P2D) model [17–19] is the most representative physics-based electrochemical model, consisting of four coupled partial differential equations (PDEs) that describe the battery behavior. The P2D model remains appropriate for applications requiring spatially resolved internal distributions, including electrode design and charging-protocol development [5,6]. However, its high computational cost and numerical instability limit its use in real-time and simulation-intensive applications [20–24].

Significant research efforts have been conducted toward developing reduced-order models of the P2D model to reduce computational burden while preserving predictive accuracy [25–27]. In particular, the Single Particle Model (SPM) is one of the most widely adopted reduced-order representations of the P2D model [28–31]. The SPM represents each electrode by a single representative spherical particle, whose surface reaction represents the electrode-averaged electrochemical reaction. Consequently, the interfacial current density is spatially uniform within each electrode. This simplification significantly reduces computational cost compared to the P2D model, which solves diffusion equations for spatially distributed particles along the electrode thickness direction, while retaining essential lithium diffusion within solid particles [29,32]. This computational advantage makes the SPM one of the physics-based options suited to real-time applications. However, the SPM neglects electrolyte dynamics, limiting its accuracy under high C-rate conditions.

Several studies have incorporated electrolyte dynamics into the SPM to improve voltage prediction accuracy across a wider range of operating conditions. Rahimian et al. [33] applied polynomial approximation to develop an SPM that incorporates full electrolyte dynamics, reducing the P2D model to a system of only 13 Differential-Algebraic Equations (DAEs) while maintaining a cell voltage error of less than 1% even under high C-rate conditions (up to 5C). The model was implemented using COMSOL, resulting in a computational speed improvement of approximately 5–6 times compared to the P2D model across discharge and charge conditions. Tanim et al. [34] incorporated electrolyte dynamics into the SPM through Laplace transformation for temporal dynamics and Integral Method Analysis-based polynomial approximation for spatial discretization, achieving voltage accuracy within 5% of the GT-AutoLion reference model [35] under various temperatures and C-rates. Notably, their model achieved computational performance comparable to conventional SPM despite incorporating full electrolyte dynamics in MATLAB. Although these SPM variants improve accuracy, they still require several seconds of computation time, which makes them unsuitable for time-critical applications such as real-time control, large-scale parameter identification, and machine learning dataset generation [33,34,36–39].

Various numerical reduction strategies have been applied to SPM variants to improve computational performance for practical applications. Marquis et al. [40] applied asymptotic analysis and the Finite Volume Method (FVM) to reduce the DAE system of the P2D model from 1120 to 110 Ordinary Differential Equations (ODEs), deriving the SPMe model. Their implementation in the PyBaMM framework, utilizing SUNDIALS DAE solvers, achieved an RMSE of 3.04 mV at 1C with a computational time of approximately 600 ms under discharge [41,42]. Subramaniam et al. [43] proposed a reduced order model similar to the SPM by volume-averaging the electrode and separator regions instead of discretizing them spatially. This approach reduced the system from approximately 1000 DAEs in the P2D model to only 15 DAEs, demonstrating voltage prediction accuracy below 5 mV at 1C compared to the P2D model. The model was solved using Implicit Differential-Algebraic solver [42,44–46] from the SUNDIALS package, achieving a computation time of 2.1 ms at 1C discharge, representing approximately 700 times speed improvement over the P2D model. While these models have achieved computational improvements, they fundamentally rely on

solvers that require numerical iterations at each time step, limiting further speed enhancement. Iterative methods employing numerical techniques such as Newton's method can suffer from numerical instability and convergence issues, which are often more problematic than computational speed or accuracy limitations [23].

Therefore, solving the physics-based models in a non-iterative manner offers an alternative with wider applicability across diverse operating conditions and real-time applications. Mehta et al. [47] proposed an SPM using polynomial approximation and semi-analytical solutions and solved the SPM non-iteratively. Their model achieved five times higher voltage accuracy than conventional SPM, requiring approximately 80 ms for a 5C discharge. However, Mehta et al. solved the DAE system in an explicit manner, which limits the choice of the time step size to satisfy the Courant number below unity. Li et al. [48] proposed a reduced order model similar to the SPM by reducing the DAE system to only 5 ODEs in state-space formulation. This non-iterative state-space formulation eliminates convergence iterations and achieved computation times of approximately 20 ms across various current profiles in MATLAB. These non-iterative models successfully converted thousands of DAE systems to a small number of ODEs. However, both models showed large voltage deviations, exhibiting RMSE of approximately 30 mV at 5C for Mehta et al. [47] and 30 mV at 2C for Li et al. [48] compared to the P2D model. Furthermore, these models were derived based on the assumption of constant electrolyte properties (i.e., electrolyte conductivity and electrolyte diffusivity), which limits their general applicability since actual electrolyte behavior in lithium-ion batteries varies significantly with electrolyte concentration.

Given these limitations, while non-iterative approaches avoid numerical instability issues, the use of constant electrolyte properties in on-board BMS implementation leads to inaccurate voltage control, potentially causing battery mismanagement and safety risks [49]. In addition, parameter identification results in inaccurately predicted physical parameters [38,50]. Therefore, there is a need to develop a non-iterative solution method for physics-based lithium-ion battery models considering the variable electrolyte properties, which also offers high computational speed.

In this work, we propose a non-iterative method to solve the Single Particle Model with electrolyte dynamics (SPMe). Physical properties are updated explicitly using values from the previous time step. Then, the one-dimensional concentration profiles for the active materials are solved using the finite volume method (FVM) with the first-order implicit scheme. Since the coefficients and boundary conditions are fixed, the system can be solved directly by the TDMA without requiring iterations. In particular, we apply an effective diffusion length, the length that the discrete gradient matches the tangent gradient at the electrode-separator interface (distinct from the physical node-to-interface distance), to simplify the ion transport in the electrolyte as a simple 3x3 matrix problem. The proposed method does not introduce a new numerical scheme for the individual governing equations. The contribution of this work is the order in which these equations are computed, allowing the SPMe to be solved without iteration. We compare the SPMe of this study against the PyBaMM SPMe [40,41] and the P2D reference model [23,51]. The results show significantly reduced computation time and consistent accuracy compared to the PyBaMM SPMe across various current and temperature conditions.

2. Method description

2.1. Overall computational framework

The P2D model is described by the following governing equations: Species conservation in the electrolyte:

$$\varepsilon_e \frac{\partial c_e}{\partial t} = \frac{\partial}{\partial x} \left(D_e^{\text{eff}} \frac{\partial c_e}{\partial x} \right) + \frac{(1 - t_+^0)}{F} j^{\text{Li}} \quad (1)$$

Species conservation in the active material:

$$\frac{\partial c_s}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_s^{\text{eff}} r^2 \frac{\partial c_s}{\partial r} \right) \quad (2)$$

Charge conservation in the electrolyte:

$$0 = \frac{\partial}{\partial x} \left(\kappa_s^{\text{eff}} \frac{\partial \phi_e}{\partial x} \right) + \frac{\partial}{\partial x} \left(\kappa_D^{\text{eff}} \frac{\partial \ln c_e}{\partial x} \right) + j^{\text{Li}} \quad (3)$$

Charge conservation in the electrode:

$$0 = \frac{\partial}{\partial x} \left(\sigma_s^{\text{eff}} \frac{\partial \phi_s}{\partial x} \right) - j^{\text{Li}} \quad (4)$$

The effective electrolyte transport properties in each region are defined by the Bruggeman correlation:

$$D_e^{\text{eff}} = D_e \epsilon_e^p, \kappa^{\text{eff}} = \kappa \epsilon_e^p \quad (5)$$

where D_e is the electrolyte diffusivity, κ is the electrolyte conductivity, ϵ_e is the porosity, and p is the Bruggeman exponent. These properties vary across the negative electrode, separator, and positive electrode regions. The parameters and boundary conditions for these governing equations are detailed in Refs. [17–19,51].

The P2D model describes lithium-ion migration and diffusion in the x-direction throughout the entire domain, electronic migration within each electrode, and radial lithium diffusion within the representative particles of each electrode. As Eqs. (1)–(4) are coupled through the current density j^{Li} , the model requires iterative solutions at each time step. Furthermore, solving Eq. (2) for every particle across the electrode thickness imposes a significant computational burden. Fig. 1a shows a schematic of the P2D model with multiple particles distributed along the electrode thickness direction. A schematic of the SPM is shown in Fig. 1b. In the SPM, each electrode has a single representative particle. This reduction allows solving the radial lithium concentration for only a single particle to represent the electrode behavior. Fig. 1c and d show

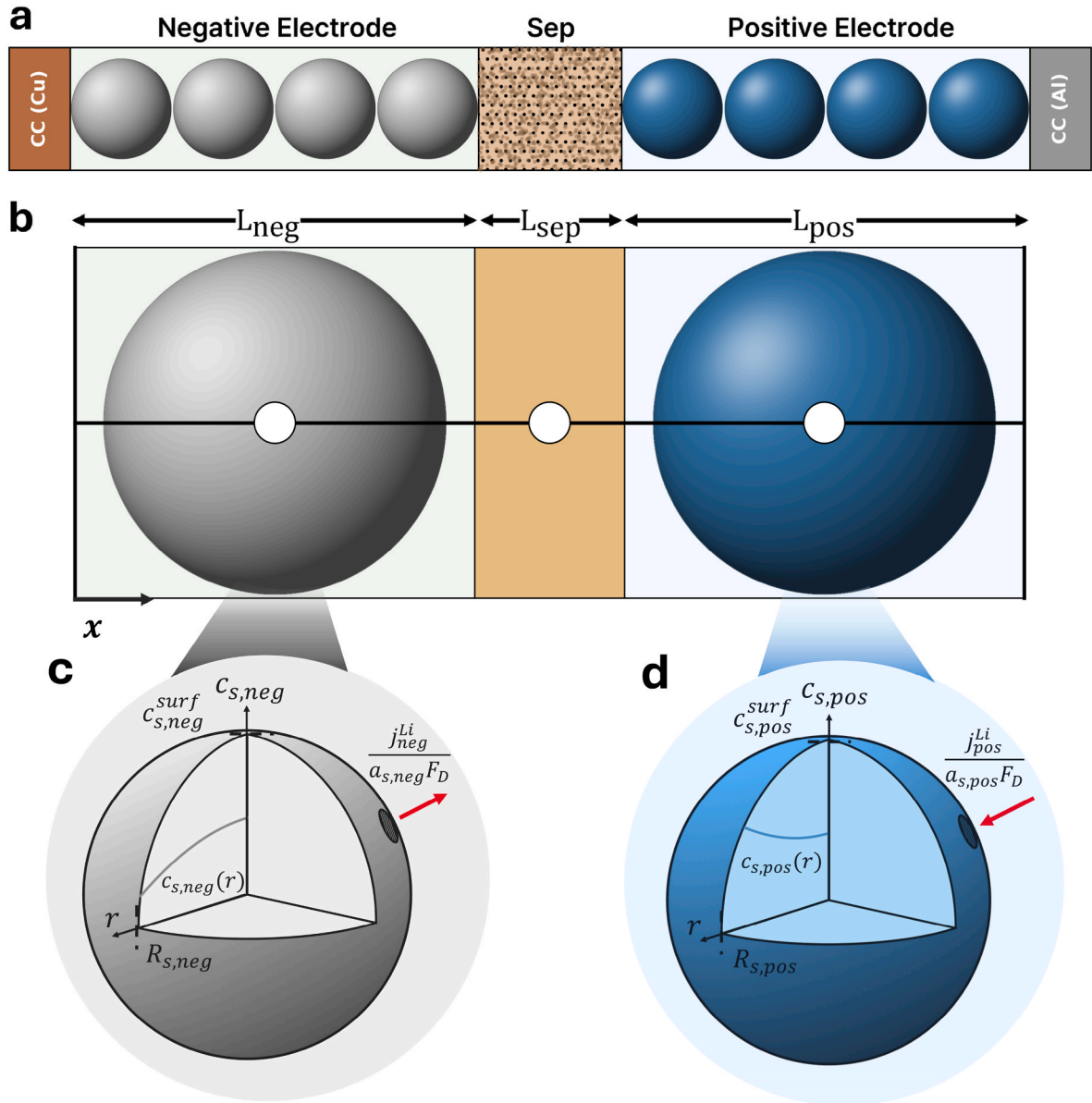


Fig. 1. (a) Schematic representation of the P2D model, and (b) computational domain of the SPM, divided into three regions with thicknesses L_{neg} , L_{sep} , and L_{pos} representing the negative electrode, separator, and positive electrode, respectively. The lithium concentration gradient profiles resulting from diffusive flux in the representative particles during discharge are shown for the (c) negative and (d) positive electrode particles.

the radial lithium concentration profiles within the single particle and diffusive fluxes at the particle surface for the negative and positive electrodes, respectively. The SPMe accounts for electrolyte dynamics while retaining the single-particle framework and spatially uniform interfacial current-density assumption of the SPM. This model assumption is not introduced by the proposed method.

The overall computational framework of the non-iterative method introduced in this work for solving SPMe is illustrated in Fig. 2. Unlike conventional iterative approaches that solve all the equations simultaneously, the present method follows a sequential calculation flow. As seen in Fig. 2, the proposed approach follows the classical numerical techniques of the FVM [52] and the key idea is to obtain the two key variables first, lithium concentrations in active materials and the electrolyte concentrations, which are required to obtain the overpotentials as well as electrolyte potentials. Since they are physical concentrations that must be positive, the two variables are solved in an implicit manner

$$\left(\underbrace{\frac{\varepsilon_{e,neg} \Delta V_{neg}}{\Delta t} + \frac{D_{e,neg/sep}^{eff} A_{neg/sep}}{\Delta x_{neg,e} + \Delta x_{sep,w}}}_{a_{c,neg}} \right) \overline{c_{e,neg}} - \underbrace{\frac{D_{e,neg/sep}^{eff} A_{neg/sep}}{\Delta x_{neg,e} + \Delta x_{sep,w}}}_{a_{e,neg}} \overline{c_{e,sep}} = \left(\underbrace{\frac{\varepsilon_{e,neg} \Delta V_{neg}}{\Delta t} \overline{c_{e,neg}^0}}_{b_{neg}} + \frac{(1 - t_+^0)}{F} \overline{j_{Li}^{neg} \Delta V_{neg}} \right) \quad (6)$$

• Separator:

$$\underbrace{\frac{D_{e,neg/sep}^{eff} A_{neg/sep}}{\Delta x_{sep,w} + \Delta x_{neg,e}} \overline{c_{e,neg}}}_{a_{w,sep}} + \left(\underbrace{\frac{D_{e,neg/sep}^{eff} A_{neg/sep}}{\Delta x_{sep,w} + \Delta x_{neg,e}} + \frac{\varepsilon_{e,sep} \Delta V_{sep}}{\Delta t} + \frac{D_{e,sep/pos}^{eff} A_{sep/pos}}{\Delta x_{sep,e} + \Delta x_{pos,w}}}_{a_{c,sep}} \right) \overline{c_{e,sep}} = \underbrace{\frac{D_{e,sep/pos}^{eff} A_{sep/pos}}{\Delta x_{sep,e} + \Delta x_{pos,w}} \overline{c_{e,sep}}}_{a_{e,sep}} = \underbrace{\frac{\varepsilon_{e,sep} \Delta V_{sep}}{\Delta t} \overline{c_{e,sep}^0}}_{b_{sep}} \quad (7)$$

(the first-order backward Euler implicit scheme is employed in this work). Note that the solution procedure of the two variables does not require numerical iterations, since the equations are one-dimensional and the matrices are tri-diagonal. The transport properties (such as electrolyte conductivity and diffusivity) are obtained in an explicit manner considering they vary slowly in time. For ease of reproducibility, the following subsections describe the details of the discretization and solution procedure, starting with the numerical discretization of the species conservation equation in the electrolyte.

2.2. Species conservation in the electrolyte

As shown in Fig. 2, the electrolyte concentration is determined by solving a compact 3×3 matrix system, which reduces numerical complexity. To obtain the electrolyte concentration by formulating the mass conservation in the electrolyte as a simple 3×3 matrix, we adopt a FVM-based 1D grid structure in the x-direction [53]. For the spatial discretization of the electrolyte concentration in the x-direction, the proposed method employs a single representative node for each of the three regions: the negative electrode, separator, and positive electrode. Consequently, it represents a single representative electrolyte concentration in each region rather than a spatially varying distribution. Fig. 1b shows the SPM computational domain discretized using the FVM with a single node for each region. The electrolyte transport properties, such as electrolyte diffusivity (D_e) and electrolyte conductivity (κ), are not treated as constant values. Rather, they are updated at each time step as functions of the local electrolyte concentration (c_e).

The FVM discretization of Eq. (1) for each region is as follows:

• Negative electrode:

• Positive electrode:

$$\underbrace{\frac{D_{e,sep/pos}^{eff} A_{sep/pos}}{\Delta x_{sep,e} + \Delta x_{pos,w}} \overline{c_{e,sep}}}_{a_{w,pos}} + \left(\underbrace{\frac{D_{e,sep/pos}^{eff} A_{sep/pos}}{\Delta x_{sep,e} + \Delta x_{pos,w}} + \frac{\varepsilon_{e,pos} \Delta V_{pos}}{\Delta t}}_{a_{c,pos}} \right) \overline{c_{e,pos}} = \left(\underbrace{\frac{\varepsilon_{e,pos} \Delta V_{pos}}{\Delta t} \overline{c_{e,pos}^0}}_{b_{pos}} + \frac{(1 - t_+^0)}{F} \overline{j_{Li}^{pos} \Delta V_{pos}} \right) \quad (8)$$

In Eqs. (6)–(8), the subscripts w and e denote the direction from the current node to the west and east interfaces, respectively. The discretization volumes without these subscripts, such as ΔV_{neg} , ΔV_{sep} , and ΔV_{pos} , represent the control volume of each region, which corresponds to the volume of the negative electrode, separator, and positive electrode, respectively. The notation with a slash, such as $D_{e,neg/sep}^{eff}$ represents the effective electrolyte diffusivity at the interface between the negative electrode and separator. The effective electrolyte diffusivity at the interface is calculated using the harmonic mean to keep the flux continuous across the interface. These diffusivity values are evaluated explicitly using the electrolyte concentration from the previous time step, allowing for a direct solution without iterative procedures. For example, at the negative electrode-separator interface:

$$D_{e,neg/sep}^{eff} = \frac{\Delta x_{neg,e} + \Delta x_{sep,w}}{\frac{\Delta x_{neg,e}}{D_{e,neg}^{eff}} + \frac{\Delta x_{sep,w}}{D_{e,sep}^{eff}}} \quad (9)$$

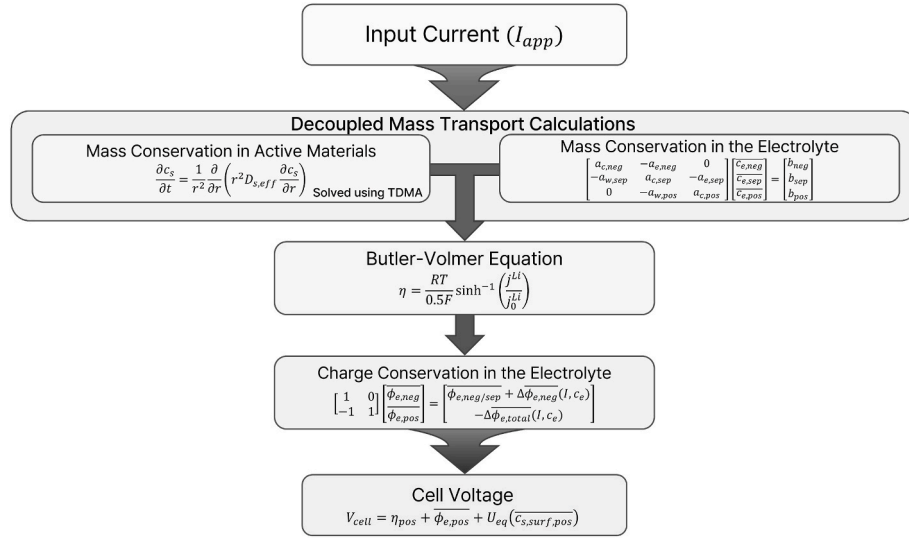


Fig. 2. Computational flowchart of the proposed method for solving SPMe. Using the applied current (I_{app}) as input, the method obtains the cell voltage sequentially without iteration. The solid-phase surface lithium concentration ($c_{s,surf}$) and electrolyte concentration (c_e) needed for the Butler-Volmer equation are obtained independently and determine electrode overpotentials and electrolyte potential in the negative electrode. Finally, the cell voltage can be determined.

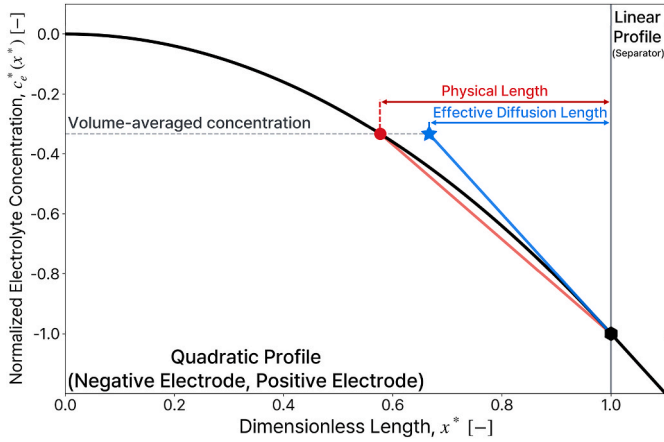


Fig. 3. Normalized quadratic electrolyte concentration profile in the electrode and separator regions, illustrating the comparison between physical and effective diffusion lengths. Although both nodes represent the volume-averaged concentration of the electrode, the red line shows a discrete gradient based on the physical diffusion length, which fails to match the actual tangent gradient at the interface. In contrast, the blue line represents the discrete gradient using the effective diffusion length by placing the node at a distance of 1/3 of the electrode thickness from the interface. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

where $\Delta x_{neg,e}$ is the discretization length from the negative electrode node to the east interface, and $\Delta x_{sep,w}$ is the discretization length from the separator node to the west interface.

Under steady-state conditions, the uniform current density assumption within each electrode yields a quadratic electrolyte concentration distribution in the electrode regions and a linear distribution in the separator. This profile is utilized solely to determine the optimal node locations for FVM discretization, rather than as a polynomial approximation for solving the electrolyte concentration. For a quadratic electrolyte concentration profile, the volume-averaged electrolyte concentration is located at $1/\sqrt{3}$ (≈ 0.577) of the electrode thickness from the current collector boundary, corresponding to the Gauss quad-

rate point. The grey dashed line in Fig. 3 represents this volume-averaged electrolyte concentration.

When multiple control volumes are used for discretization, uniform grid spacing is typically employed [54]. However, when each region is represented by a single control volume, the node location significantly affects the accuracy [55,56]. Therefore, the representative node must be selected such that the discrete gradient between the node in each region and the electrode-separator interface matches the tangent gradient of the concentration profile at the electrode-separator interface. If the discretization node is chosen at the volume-averaged concentration location, the discrete gradient does not match the tangent gradient at the interface, as shown by the red line in Fig. 3. To ensure that the discrete gradient equals the tangent gradient at the interface while preserving the volume-averaged electrolyte concentration, the node for proper discretization must be located at 1/3 of the electrode thickness from the electrode-separator interface. This location, illustrated by the blue line in Fig. 3, provides accurate gradient matching at the interface.

Consequently, the length from this location to the electrode-separator interface is defined as the effective diffusion length, which enables accurate flux calculation and yields a physically consistent electrolyte concentration profile. This effective length is used in the flux discretization terms in Eqs. (6)–(8), corresponding to $\Delta x_{neg,e}$ and $\Delta x_{pos,w}$.

The coefficients of the discretized equations for electrolyte concentration form a 3×3 tridiagonal matrix, which can be expressed in matrix form as follows:

$$\begin{bmatrix} a_{c,neg} & -a_{e,neg} & 0 \\ -a_{w,sep} & a_{c,sep} & -a_{e,sep} \\ 0 & -a_{w,pos} & a_{c,pos} \end{bmatrix} \begin{bmatrix} \overline{c_{e,neg}} \\ \overline{c_{e,sep}} \\ \overline{c_{e,pos}} \end{bmatrix} = \begin{bmatrix} b_{neg} \\ b_{sep} \\ b_{pos} \end{bmatrix} \quad (10)$$

2.3. Species conservation in the active material

As presented in Fig. 2, the mass conservation in the active material is performed as part of the decoupled mass transport calculations. Eq. (2) is solved numerically using FVM based on the half control volume method proposed by Patankar [52]. Detailed descriptions of the numerical discretization and formulation are provided in Ref. [23]. Furthermore, while that work utilized uniform numerical discretization, the present study adopts non-uniform control volumes for discretization, with finer

resolution toward the particle surface. The spacing between adjacent nodes decreases by a factor of 0.83 toward the particle surface.

Applying FVM to Eq. (2), the discretized equation for an interior particle node ($k < n$) is:

$$\underbrace{\frac{D_{s,k-\frac{1}{2}}^{eff} A_{k-\frac{1}{2}}}{\Delta r_{w,k}}}_{a_{w,k}} c_{s,k-1} + \left(\underbrace{\frac{D_{s,k-\frac{1}{2}}^{eff} A_{k-\frac{1}{2}}}{\Delta r_{w,k}} + \frac{\Delta V_k}{\Delta t} + \frac{D_{s,k+\frac{1}{2}}^{eff} A_{k+\frac{1}{2}}}{\Delta r_{e,k}}}_{a_{c,k}} \right) c_{s,k} - \underbrace{\frac{D_{s,k+\frac{1}{2}}^{eff} A_{k+\frac{1}{2}}}{\Delta r_{e,k}}}_{a_{e,k}} c_{s,k+1} = \underbrace{\frac{\Delta V_k c_{s,0}^0}{\Delta t}}_{a_{t,k}} \quad (11)$$

At the particle surface ($k = n$):

$$\underbrace{\frac{D_{s,k-\frac{1}{2}}^{eff} A_{k-\frac{1}{2}}}{\Delta r_{w,k}}}_{a_{w,k}} c_{s,k-1} + \left(\underbrace{\frac{D_{s,k-\frac{1}{2}}^{eff} A_{k-\frac{1}{2}}}{\Delta r_{w,k}} + \frac{\Delta V_k}{\Delta t}}_{a_{c,k}} \right) c_{s,k} = \underbrace{\frac{\Delta V_k c_{s,0}^0}{\Delta t}}_{a_{t,k}} c_{s,k} - \frac{\bar{j} \bar{l}}{a_s F} A_k \quad (12)$$

In the above equations, $A_{k-\frac{1}{2}}$ and $A_{k+\frac{1}{2}}$ represent the interface areas at the west and east faces, $\Delta r_{w,k}$ and $\Delta r_{e,k}$ are the radial distances to the adjacent nodes in the west and east directions, respectively, and ΔV_k is the volume of the control volume at node k . At the particle surface, A_k represents the face area of the boundary control volume.

Finally, these discretized equations are arranged into the following tridiagonal matrix system:

$$\begin{bmatrix} a_{c,0} & -a_{e,0} & 0 & \cdots & 0 & 0 & 0 \\ -a_{w,1} & a_{c,1} & -a_{e,1} & \cdots & 0 & 0 & 0 \\ 0 & -a_{w,2} & a_{c,2} & -a_{e,2} & 0 & 0 & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & 0 & 0 & -a_{w,n-2} & a_{c,n-2} & -a_{e,n-2} & 0 \\ 0 & 0 & 0 & \cdots & -a_{w,n-1} & a_{c,n-1} & -a_{e,n-1} \\ 0 & 0 & 0 & \cdots & 0 & -a_{w,n} & a_{c,n} \end{bmatrix} \begin{bmatrix} c_{s,0} \\ c_{s,1} \\ c_{s,2} \\ \vdots \\ c_{s,n-2} \\ c_{s,n-1} \\ c_{s,n} \end{bmatrix} = \begin{bmatrix} a_{t,0} c_{s,0}^0 \\ a_{t,1} c_{s,1}^0 \\ a_{t,2} c_{s,2}^0 \\ \vdots \\ a_{t,n-2} c_{s,n-2}^0 \\ a_{t,n-1} c_{s,n-1}^0 \\ a_{t,n} c_{s,n}^0 - A_n \frac{\bar{j} \bar{l}}{a_s F} \end{bmatrix} \quad (13)$$

2.4. Charge conservation in the electrolyte

Although Fig. 2 illustrates the sequential flow from the Butler-Volmer equation to the electrolyte potential, the final cell voltage is determined through the overpotential relationship detailed in Section 2.5. Since this calculation requires electrolyte potential as a preliminary variable, this section provides the analytical solution for the potential distribution to determine the electrolyte potential at the positive electrode. Under the assumption of constant current density within each electrode, Eq. (3) can be reformulated by expressing the diffusional

conductivity κ_D^{eff} in terms of κ^{eff} :

$$\frac{\partial}{\partial x} \left(\kappa^{eff} \frac{\partial \phi_e^*}{\partial x} \right) + j^{Li} = 0 \quad (14)$$

where ϕ_e^* represents the modified electrolyte potential defined as [57]:

$$\phi_e^* = \phi_e + \frac{2RT}{F} (t_+^0 - 1) \left(1 + \frac{d \ln f_{\pm}}{d \ln c_e} \right) \ln \frac{c_e}{c_{e,0}} \quad (15)$$

where $c_{e,0}$ is the initial electrolyte concentration and $d \ln f_{\pm} / d \ln c_e$ relates to the thermodynamic factor.

Solving Eq. (14) analytically reveals that the electrolyte potential follows a quadratic polynomial in x within the electrodes, while varying linearly in the separator. As discussed in Section 2.2, the volume-averaged value in each electrode is given by the value at $1/\sqrt{3}$ of the electrode thickness from the current collector boundary. Therefore, the electrolyte potential difference between these volume-averaged locations effectively represents the characteristic electrolyte potential drop across the cell. By solving Eq. (14) and applying Eq. (15) at the volume-averaged node locations, the electrolyte potential difference between the electrodes can be expressed as:

$$\overline{\phi_{e,pos}} = \overline{\phi_{e,neg}} - I_{app} \left(\frac{L_{neg}}{3\kappa_{neg}^{eff}} + \frac{L_{sep}}{\kappa_{sep}^{eff}} + \frac{L_{pos}}{3\kappa_{pos}^{eff}} \right) + \frac{2RT}{F} (t_+^0 - 1) \left(1 + \frac{d \ln f_{\pm}}{d \ln c_e} \right) \ln \frac{\overline{c_{e,pos}}}{\overline{c_{e,neg}}} \quad (16)$$

The absolute electrolyte potential at the negative electrode is obtained from the Butler-Volmer equation, as detailed in Section 2.5.

2.5. Butler-Volmer equation

When the anodic and cathodic transfer coefficients are both 0.5, the Butler-Volmer equation can be expressed as:

Table 1

Physical parameters used for the SPMe (this study, PyBaMM), and the P2D model. The same parameters were used in all models. Electronic conductivity is not required by the SPMe solved using the proposed method. The HPPC simulations use the initial stoichiometry specified for driving profiles, and the MSCC simulations use the initial stoichiometry specified for charge.

Parameter	Negative Electrode	Separator	Positive Electrode	Reference
Thickness [μm]	73.5	25	70	[23]
Initial porosity, ϵ_e [–]	0.4382	0.43	0.3	[23]
Bruggeman factor, p [–]	1.5	1.5	1.5	[23]
Diffusivity of solid active materials at 298 K, $D_{s,\text{ref}}$ [m^2/s]	5.5E-14	–	1.0E-14	[23]
E_a for diffusivity of solid active material [J/mol]	4000	–	20000	[23]
Maximum concentration of solid active materials, $c_{s,\text{max}}$ [mol/ m^3]	30555	–	51555	[23]
Initial stoichiometry of solid active materials for discharge, $x_{100\%}$ [–]	0.756	–	0.465	[23]
Initial stoichiometry of solid active materials for charge, $x_{0\%}$ [–]	0.05	–	0.95	[23]
Initial stoichiometry of solid active materials for driving profiles, x [–]	0.756	–	0.465	*ad
Particle radius, R_s [μm]	12.5	–	8.5	[23]
Film resistance [Ωm^2]	0.023	–	0.023	[23], *ad
Rate constant for electrochemical reactions at 298 K, k_0 [$\text{m}^{2.5}\text{mol}^{-0.5}\text{s}^{-1}$]	1.764E-11	–	6.667E-11	[23]
E_a for rate constant [J/mol]	30000	–	30000	[23]
Electronic conductivity for the SPMe (PyBaMM) and the P2D model, σ [S/m]	1000	–	1000	*ad
Equilibrium Potential, U_{eq} [V]	Kim et al.	–	Kim et al.	[23]
Lithium-ion transference number in the electrolyte, t_e^0 [–]	0.435	–	–	[23]
Thermodynamic factor, $\partial \ln f_{\pm} / \partial \ln c_e$ [–]	0	–	–	[23]
Initial electrolyte concentration, $c_{e,0}$ [mol/ m^3]	1000	–	–	[23]
Electrolyte diffusivity, D_e [m^2/s]	$4.615 \times 10^{-10} \exp \left[-\frac{23935.74}{8.314} \left(\frac{1}{T} - \frac{1}{298.14} \right) - 6.14 \times 10^{-4} c_e \exp \left(\frac{2311.72}{8.314} \left(\frac{1}{T} - \frac{1}{298.14} \right) \right) \right]$			*ad
Electrolyte conductivity, κ [S/m]	$3.334 \times 10^{-3} c_e \exp \left[-\frac{7794.35}{8.314} \left(\frac{1}{T} - \frac{1}{298.14} \right) - 1.074 \times 10^{-3} c_e \exp \left(\frac{5822.4}{8.314} \left(\frac{1}{T} - \frac{1}{298.14} \right) \right) \right]$			*ad
Cell capacity per active area [Ah/ m^2]	19.667	–	–	[23]

*ad: Adjusted in this study.

$$j^{Li} = a_s k F (c_{s,\text{max}} - c_{s,\text{surf}})^{0.5} c_{s,\text{surf}}^{0.5} c_e^{0.5} \sinh \left(\frac{0.5F}{RT} \eta \right) \quad (17)$$

where the overpotential η is defined as:

$$\eta = \phi_s - \phi_e - U_{\text{eq}}(c_{s,\text{surf}}) - \frac{R_{\text{film}} j^{Li}}{a_s} \quad (18)$$

Here, R_{film} is the film resistance, a_s is the specific surface area, U_{eq} is the equilibrium potential, and k is the rate constant for electrochemical reactions.

In Eq. (18), both the overpotential η and current density j^{Li} are implicitly coupled, which typically requires an iterative convergence process at each time step. However, by assuming spatially uniform current density within each electrode, the overpotential can be explicitly determined without iteration as follows:

$$\bar{\eta} = \frac{RT}{0.5F} \sinh^{-1} \left(\frac{\bar{j}^{Li}}{a_s k F (c_{s,\text{max}} - c_{s,\text{surf}})^{0.5} c_{s,\text{surf}}^{0.5} c_e^{0.5}} \right) \quad (19)$$

The electrolyte concentration $\bar{c}_e$ and the solid-phase surface lithium concentration $\bar{c}_{s,\text{surf}}$ are obtained from Eq. (10) and Eq. (13), respectively. The spatially averaged current density $\bar{j}^{Li}$ in each electrode is calculated from:

$$\bar{j}^{Li} = \frac{1}{L} \int_0^L j^{Li} dx = \frac{I}{A \cdot L} \quad (20)$$

where I is the current, A is the electrode cross-sectional area, and L is the electrode thickness.

Since the overpotential in each electrode is known from Eq. (19), the electrolyte potential in the negative electrode can be expressed by rearranging Eq. (18):

$$\bar{\phi}_{e,\text{neg}} = \bar{\phi}_{s,\text{neg}} - \left(\bar{\eta}_{\text{neg}} + U_{\text{eq}}(c_{s,\text{surf},\text{neg}}) + \frac{R_{\text{film},\text{neg}} \bar{j}^{Li}}{a_{s,\text{neg}}} \right) \quad (21)$$

Given that the solid-phase potential in the negative electrode is assumed to be 0 V (i.e., $\bar{\phi}_{s,\text{neg}} = 0$ V), the average electrolyte potential in the negative electrode ($\bar{\phi}_{e,\text{neg}}$) is directly obtained from Eq. (21). By substituting the average electrolyte potential in the negative electrode obtained from Eq. (21) into Eq. (16), the average electrolyte potential in the positive electrode ($\bar{\phi}_{e,\text{pos}}$) is determined. Because the negative electrode potential serves as the zero reference, the average solid-phase potential in the positive electrode directly corresponds to the terminal voltage of the cell. Therefore, the cell voltage can be expressed as:

$$V_{\text{cell}} = \bar{\phi}_{s,\text{pos}} = \bar{\eta}_{\text{pos}} + U_{\text{eq}}(\bar{c}_{s,\text{surf},\text{pos}}) + \bar{\phi}_{e,\text{pos}} + \frac{R_{\text{film},\text{pos}} \bar{j}^{Li}}{a_{s,\text{pos}}} \quad (22)$$

The complete solution procedure, from the applied current input to the final cell voltage calculation, is summarized in Fig. 2.

2.6. Computational details

The tridiagonal matrix systems arising from the FVM discretization of the electrolyte concentration (Eq. (10)) and solid-phase concentration (Eq. (13)) are solved using the Tri-Diagonal Matrix Algorithm (TDMA). Since the governing equations are decoupled and solved sequentially, with the transport properties evaluated explicitly from the previous time step, no iterative convergence process is required at each time step. To validate the effective diffusion length approach described in Section 2.2, we compare results obtained using effective length discretization, physical length discretization, and a model without electrolyte dynamics (i.e., constant electrolyte concentration). The SPMe solved by the

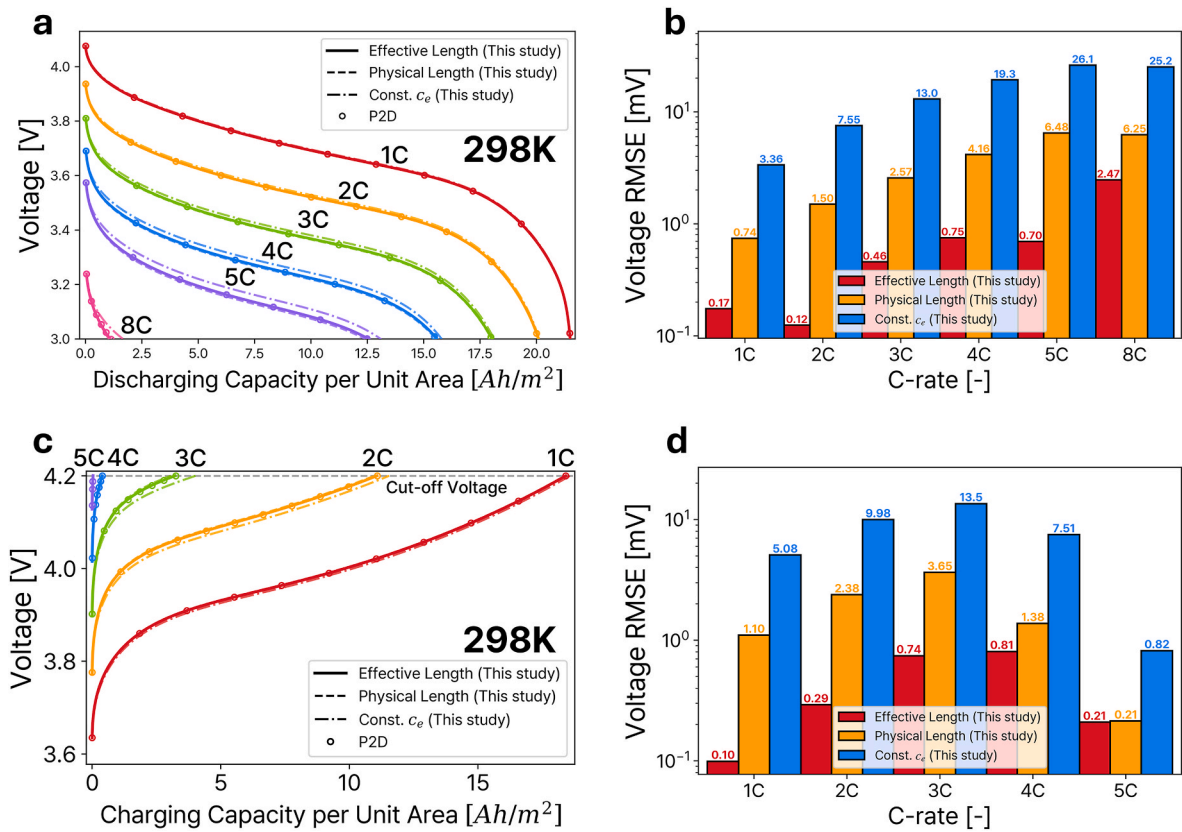


Fig. 4. Accuracy comparison of discretization approaches for SPMe against the P2D model [23] at 298 K when solving the electrolyte concentration using FVM: the effective diffusion length discretization, the physical length discretization, and the model using constant electrolyte concentration (Const. c_e). (a) Discharge voltage curves from 1C to 5C and 8C (3.0 V cut-off voltage) with (b) the corresponding voltage RMSE relative to the P2D model. (c) Charge voltage curves from 1C to 5C (4.2 V cut-off voltage) with (d) the corresponding voltage RMSE relative to the P2D model. All voltage RMSE values in (b) and (d) are displayed on a logarithmic scale.

proposed method is also compared with both the P2D model and the PyBaMM SPMe implementation [41], which uses the IDAKLU solver [45,46]. The P2D model presented by Kim et al. [23], which was validated in that work, is used as the reference model.

For spatial discretization in the x-direction, the present method uses one control volume for the negative electrode, separator, and positive electrode. In contrast, the PyBaMM SPMe uses three control volumes in each region, which is the minimum number accepted by its discretization. Simulations with fewer control volumes fail during model setup. The P2D model employs a finer mesh of 30, 20, and 30 control volumes for the negative electrode, separator, and positive electrode regions, respectively.

Regarding the radial direction within the particles, a grid independence study was performed to determine the converged number of control volumes under various temperature and current conditions. This study was conducted in two stages under full discharge, charge, and various driving profiles. In the first stage, a reference number of control volumes was established by increasing the radial discretization from 10 control volumes in increments of 5 (i.e., 10, 15, 20, ...). This process continued until the voltage RMSE between consecutive discretization control volumes fell below 0.1 mV. Subsequently, the converged number of control volumes for actual simulations was determined. Starting from 10 control volumes, the count was increased in increments of 1 until the voltage RMSE compared to the reference number of control volumes fell below 0.1 mV. For the proposed method and the P2D model, a fixed time step was used for constant-current discharging and charging, and its value was set according to the time taken to reach the cut-off voltage. A 1 s step was used when this time was on the order of tens to thousands of seconds, a 0.1 s step when it was on the order of a few to about 10 s, and

a 0.01 s step for shorter cases. For driving profiles, the 1 s sampling interval of the data was used as the time step. For the PyBaMM SPMe, which internally employs an adaptive time step scheme, results were extracted by interpolating the adaptive solution at these corresponding time steps. The voltage curves presented in the results section are obtained using these converged discretization control volumes.

For computational speed benchmarking, a time-step independence study was conducted to determine the converged time step. Based on the grid independence study results for the particle domain, time-step independence studies were conducted under various temperatures and constant current conditions. The time step interval was decreased from 30 s to 2 s in decrements of 1 s, from 2 s to 0.1 s in decrements of 0.1 s, and from 0.1 s to 0.01 s in 0.01 s decrements. Convergence was achieved when the voltage RMSE relative to the reference results obtained at a time step of 0.01 s fell below 1 mV, and this converged time step was used for benchmarking. Following the identical procedure, the time step independence study for PyBaMM was performed by adjusting the interpolation interval used to extract results from the adaptive solution, with absolute and relative tolerances set to 10^{-6} . All simulations were performed on a desktop computer equipped with an AMD Ryzen 9 7900X CPU (4.7 GHz base clock and up to 5.6 GHz boost clock), 32 GB RAM, and a 64-bit Microsoft Windows 11 operating system. The SPMe solved by the proposed method and the P2D model were implemented in C++. The PyBaMM SPMe simulations were performed using PyBaMM version 25.12.2. All three models were executed using a single CPU core.

3. Results and discussion

The model parameters used in this study are summarized in Table 1.

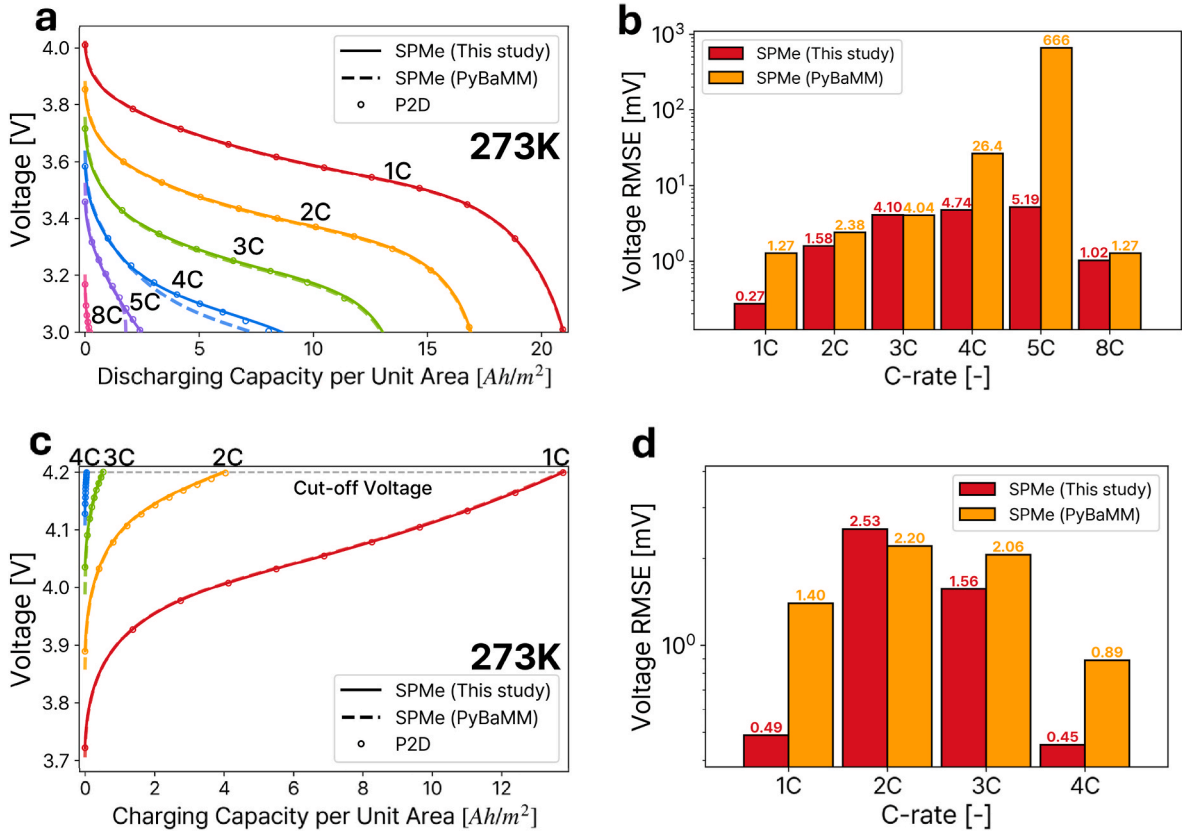


Fig. 5. Accuracy comparison of the SPMe of this study and the PyBaMM SPMe against the P2D model [23] at 273 K. (a) Discharge voltage curves from 1C to 5C and 8C (3.0 V cut-off voltage) with (b) the corresponding voltage RMSE relative to the P2D model. (c) Charge voltage curves from 1C to 4C (4.2 V cut-off voltage) with (d) the corresponding voltage RMSE relative to the P2D model. All voltage RMSE values in (b) and (d) are displayed on a logarithmic scale.

The electrolyte diffusivity and electrolyte conductivity were modeled using custom functions for a PC:EC:DMC composition of 10:27:63, and the Arrhenius-based temperature dependence of the solid-phase diffusivity D_s^{eff} and the rate constant k were consistently applied across the SPMe model of this study, the PyBaMM SPMe, and the P2D model.

3.1. Comparison of electrolyte discretization approaches

To evaluate the proposed effective length approach, we compared its accuracy with physical length discretization, and a model without electrolyte dynamics (constant c_e). Each approach was solved on its converged grid from the grid independence study. Model accuracy was assessed by calculating voltage RMSE against the P2D model at 298 K, with comprehensive comparison results presented in Fig. 4.

Fig. 4a depicts the discharge voltage profiles for C-rates ranging from 1C to 5C and 8C. The effective length discretization approach accurately represents the performance of the P2D model across all C-rates, with a voltage root mean square error (RMSE) of 0.17 mV at 1C, which slightly increases to 2.47 mV at 8C (Fig. 4b). In contrast, the physical length discretization approach exhibits an increasing deviation trend as the C-rate rises, with a voltage RMSE of 0.64 mV at 1C that escalates more significantly towards 8C. This discrepancy arises from the overestimation of the representative electrolyte concentration ($\bar{c}_e$) in each electrode region compared to the P2D model (Figs. S1–S2). Unlike the physical length discretization, the constant c_e approach underestimates voltage behavior by neglecting electrolyte dynamics, resulting in high voltage RMSE values of 26.1 mV at 5C and 25.2 mV at 8C.

Fig. 4c presents the charge voltage profiles from 1C to 5C under a 4.2 V cut-off voltage. The effective length discretization approach maintains high precision across all C-rates, with a voltage RMSE of 0.10 mV at 1C and 0.21 mV at 5C (Fig. 4d). Although the physical length

discretization approach aligns reasonably well with a voltage RMSE below 4 mV, it is less accurate than the case with effective diffusion length due to the overestimation of electrolyte concentration observed during discharge. The constant c_e approach consistently shows high voltage RMSE across all C-rates during charging, consistent with the trend observed in the discharge results. Under 5C charge conditions at 298 K, the constant c_e approach exhibits relatively low voltage RMSE, as the terminal voltage reaches the 4.2 V cut-off voltage in approximately 1 s, which results in insufficient time for electrolyte dynamics to significantly impact the voltage. Under such brief operating conditions, even the constant c_e approach can accurately predict voltage behavior.

3.2. Comparison of voltage accuracy with the PyBaMM SPMe

Beyond analysis of electrolyte discretization approaches in Section 3.1, this section compares the voltage accuracy of the SPMe of this study and the PyBaMM SPMe against the P2D model. To ensure a fair comparison, the results in Figs. 5 and 6 were also obtained using the converged number of control volumes determined through a grid independence study (Figs. S3–S5). Fig. 5 presents the results under various constant current conditions at 273 K, while Fig. 6 extends the validation to driving profiles at 248 K.

Fig. 5a and c present discharge and charge voltage curves, respectively, across a range of C-rates. Consistent with the behavior observed at 298 K in Section 3.1, the proposed method demonstrates low voltage RMSE compared to the P2D model across all operating conditions. Overall, the proposed method and the PyBaMM SPMe show similar discrepancies relative to the P2D model, except for the 4C and 5C discharges. In these conditions, the calculated electrolyte concentration in the positive electrode approaches zero ($\sim 200 \text{ mol/m}^3$) at 4C and 5C discharge, indicating severe depletion (Fig. S6).

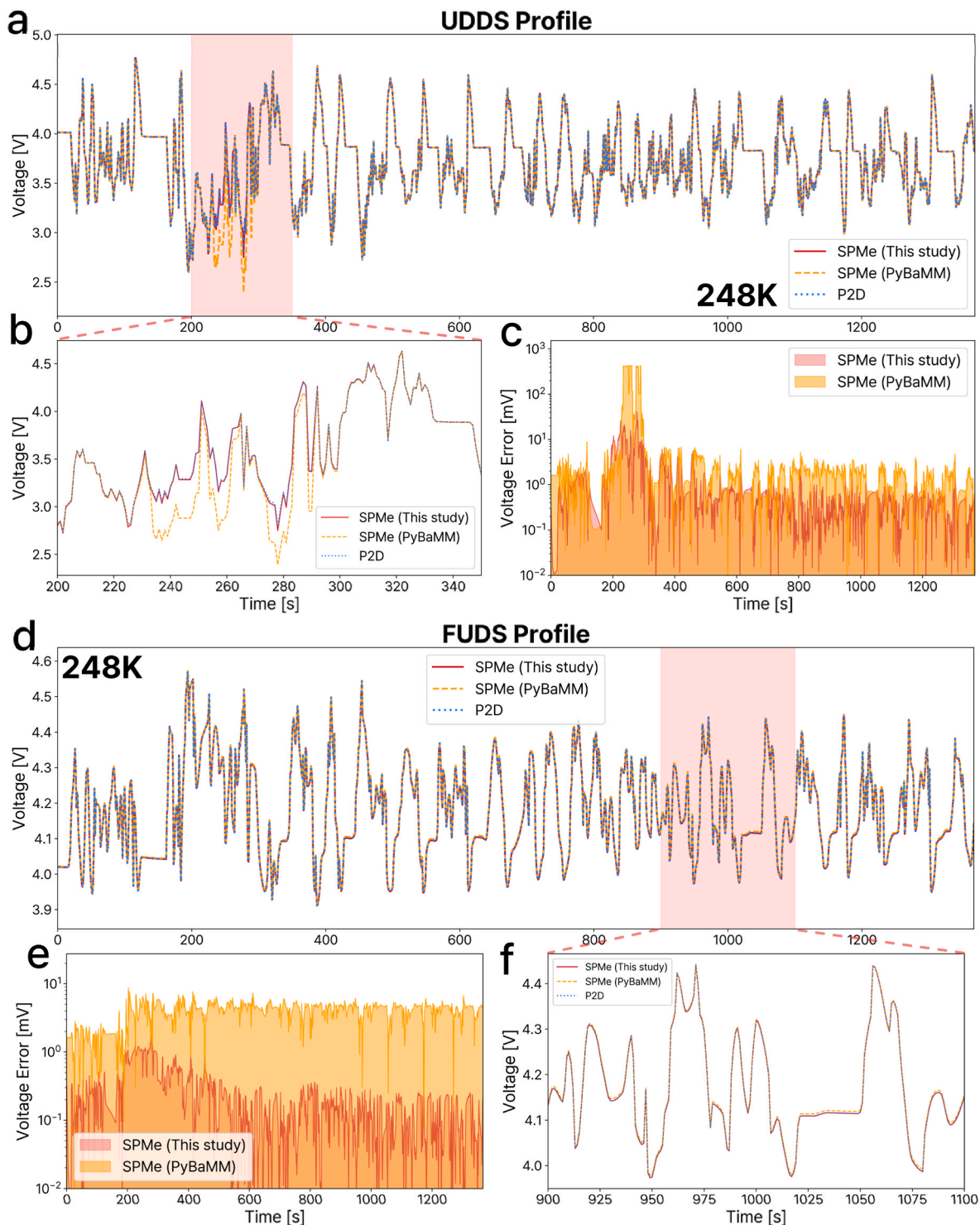


Fig. 6. Accuracy comparison of the SPMe of this study and the PyBaMM SPMe against the P2D model under driving profiles at 248 K. (a) Voltage results under the UDDS profile, with (b) a magnified view from 200 to 350 s and (c) the corresponding instantaneous voltage error on a logarithmic scale. (d) Voltage results under the FUDS profile, with (e) the corresponding instantaneous voltage error on a logarithmic scale and (f) a magnified view from 900 s to 1100 s.

During charging, both the proposed method and the PyBaMM SPMe show reasonable agreement with the P2D model from 1C to 4C, as depicted in Fig. 5c. Across all charging C-rates, both models maintain RMSE values below 2.6 mV.

The performance of models under driving profiles characterized by rapid current variations at 248 K is validated in Fig. 6. The voltage response of the SPMe of this study, the PyBaMM SPMe, and the P2D model under the UDDS (Urban Dynamometer Driving Schedule) profile

[58] is presented in Fig. 6a. Except for the localized deviations observed between 220 and 300 s in Fig. 6b, the voltage profiles generally correspond with the P2D model. The proposed method accurately tracks the P2D voltage profile, with the notable exception of the period near 280 s. In contrast, the PyBaMM SPMe exhibits substantial deviations from the P2D model starting from approximately 230 s. Within this magnified segment for the localized peak near 280 s, the maximum error of the SPMe of this study is within approximately 40 mV, whereas the PyBaMM

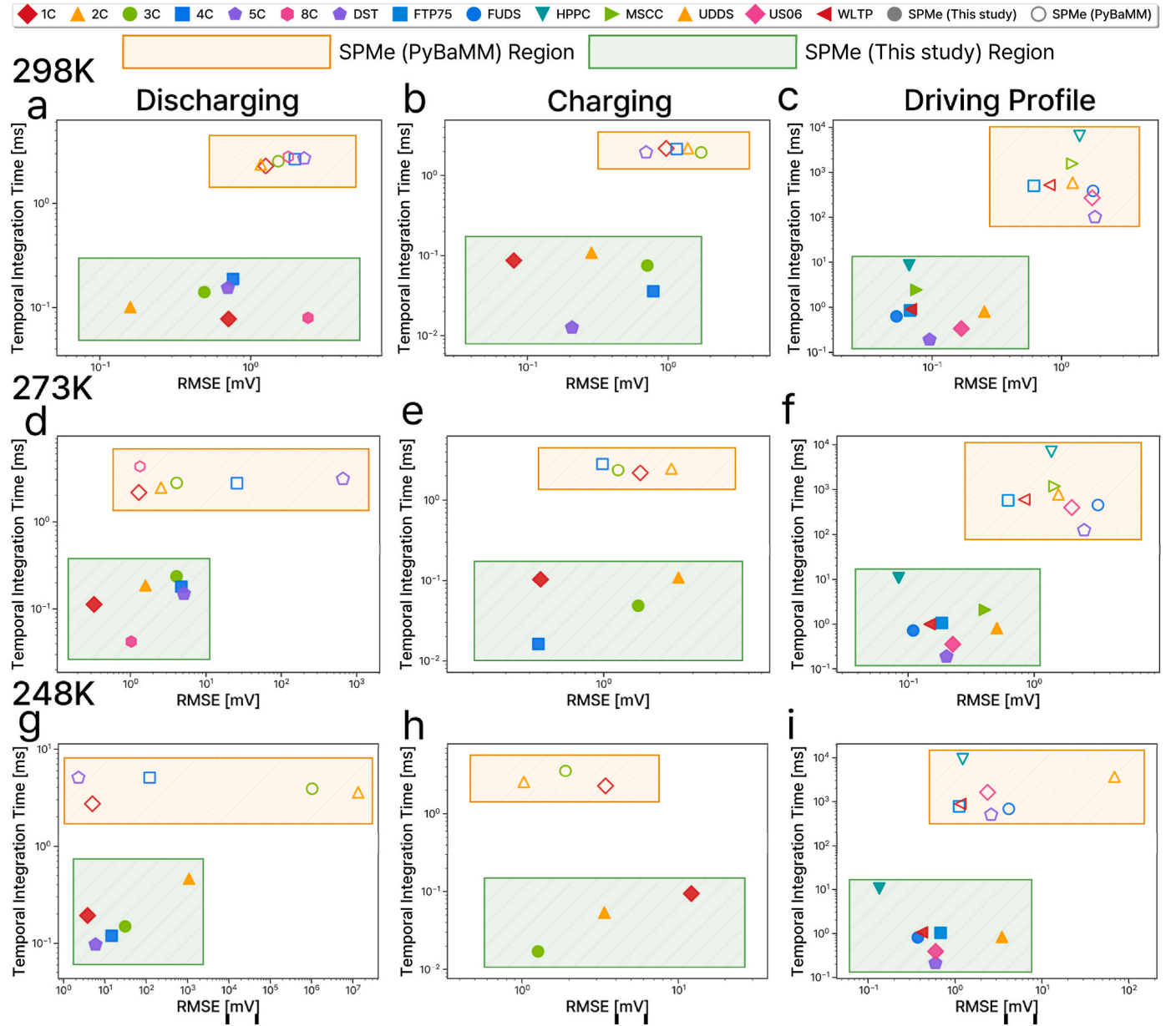


Fig. 7. Computational performance and accuracy comparison of the SPMe of this study and the PyBaMM SPMe across various temperatures. The scatter plots show the time required for the temporal integration versus voltage RMSE relative to the P2D model at (a–c) 298 K, (d–f) 273 K, and (g–i) 248 K. The subplots are organized by operating conditions: discharging (a, d, g) with a 3.0 V cut-off voltage, charging (b, e, h) with a 4.2 V cut-off voltage, and driving profiles (c, f, i) including DST, FTP75, FUDS, HPPC, MSCC, UDDS, US06, and WLTP. (a–i) x-axis and y-axis are displayed on a logarithmic scale.

SPMe produces instantaneous voltage errors on the order of several hundred mV (Fig. 6c). During these transient periods, abrupt current variations reaching up to approximately 5.5C trigger a rapid reduction and depletion in electrolyte concentration within the positive electrode.

The voltage response under the Federal Urban Driving Schedule (FUDS) profile [59,60] is presented in Fig. 6d. As shown in Fig. 6e, the differences in instantaneous voltage response indicate that errors reach several mV over the course of the profile. Fig. 6f provides the detailed view from 900 to 1100 s. Near 1020 s, where the applied current changes abruptly, both the PyBaMM SPMe and the proposed method track the P2D model response closely. The precise voltage prediction of the proposed method is attributed to the implementation of the half control volume method with non-uniform grid spacing for mass conservation in the active material. While these results show good agreement with the P2D model, we discuss the limitations of the current method in more detail in Section 3.4.

3.3. Computational performance analysis

Fig. 7 presents a comparison of voltage RMSE and computation time between the SPMe of this study and the PyBaMM SPMe at three temperatures: 298 K (Fig. 7a–c), 273 K (Fig. 7d–f), and 248 K (Fig. 7g–i). For each temperature, the performance is evaluated under constant current discharge, charge, and various driving profiles. The driving profiles encompass the Supplemental Federal Test Procedure (US06) [23], Dynamic Stress Test (DST) [59,60], FUDS [60], UDDS [58], Hybrid Pulse Power Characterization (HPPC) [61], Multi-Stage Constant Current (MSCC) profile, Worldwide Harmonized Light Vehicles Test Procedure (WLTP) [62], and Federal Test Procedure 75 (FTP75) [63]. The MSCC profile follows a practical fast-charging strategy that charges as fast as possible while avoiding lithium plating. The profile was generated once with the P2D model at 298 K. Charging starts at a constant current of 2.5C. Whenever the negative electrode potential drops to the 20 mV limit, the

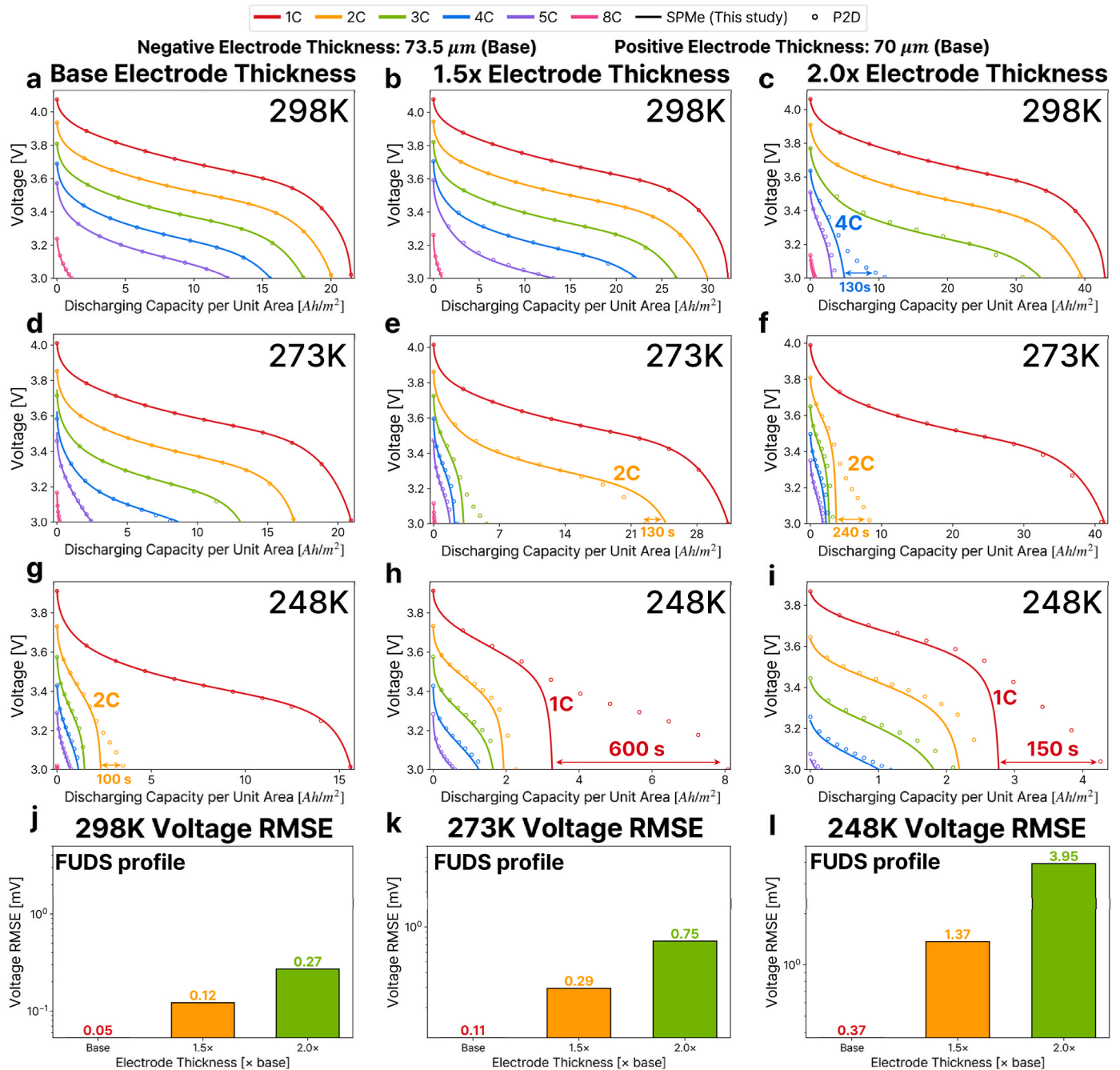


Fig. 8. Accuracy operating range over C-rate, temperature, and electrode thickness. (a–i) Constant-current discharge curves of the SPMe of this study (solid lines) and the P2D model (open circles) from 1C to 8C. Columns correspond to the base, 1.5 $\times$, and 2 $\times$ electrode thicknesses, and rows to 298 K, 273 K, and 248 K. In each row, the C-rate with the largest voltage RMSE at the 2 $\times$ thickness is marked for the three thicknesses. Arrows give the early cut-off time, the interval by which the discharge ends earlier than in the P2D model, and where no early cut-off occurs, the voltage RMSE is annotated instead. The voltage RMSE for each condition is presented in Fig. S9. (j–l) Voltage RMSE against the P2D model under the FUDS driving profile for the three thicknesses at (j) 298 K, (k) 273 K, and (l) 248 K.

current is switched to the next lower stage, for example from 2.5C to 2.0C, and charging continues at that current. The stages are spaced 0.5C apart between 2.5C and 1C, and 0.2C apart below 1C. The resulting current profile was applied identically to all three models. Fig. S8i illustrates the behavior of the lithium plating potential versus time obtained from the MSCC profile adopted in this study.

Voltage RMSE values were also calculated following the completion of the grid independence study and a subsequent time step independence study. The computation times reported in Fig. 7 represent the time required for temporal integration only (without overhead), for a fair comparison since the overhead is relatively more excessive in PyBaMM

SPMe. The time required for temporal integration of the PyBaMM SPMe is obtained from the internal option available from IDAKLU. Note that, because the IDAKLU solver uses an adaptive time step while the proposed method uses a fixed one, this is still not a direct comparison of the computational time. However, this can be useful information for PyBaMM developers and the scholars reproducing the proposed method. The total computation time of the PyBaMM SPMe and the proposed method is reported in Fig. S7.

As shown in Fig. 7a–c, which correspond to discharging, charging, and driving profiles, respectively, a clear distinction in computational performance is observed between the two results. Based on the set-up,

the proposed method is approximately 23 to 57 times faster for discharging and charging, and approximately 532 times to 797 times faster for the driving profiles. The driving profiles show more speedups, because their rapidly varying currents make the adaptive IDAKLU solver take multiple time steps, each with Newton iterations, while the proposed method uses a fixed time step. Both models exhibit good agreement with the P2D model, and the difference in voltage RMSE between them is small. In the plots, the SPMe of this study lies toward the lower-left region while the PyBaMM SPMe lies toward the upper-right region. Fig. 7d–f illustrate the performance at 273 K, showing a spatial distribution similar to that at 298 K. At 273 K, the speedup is on average about 30 times for discharging (Fig. 7d), 67 times for charging (Fig. 7e), and 710 times for the driving profiles (Fig. 7f).

Differences in computational speed are the largest at 248 K (Fig. 7g–i). Based on the time required for the temporal integration, the proposed method is on average 28 times faster for discharging (Fig. 7g), 93 times faster for charging (Fig. 7h), and about 2000 times faster for driving profiles (Fig. 7i). This gap arises partly from the fine radial grid that the PyBaMM SPMe needs for a grid-independent solution at low temperature. When the PyBaMM SPMe uses the same radial grid of 23 control volumes, at which the SPMe of this study converges, the speedup for the UDSS profile drops to about 195 times (about 1.8 ms against 348 ms). A gap of three orders of magnitude would not remain if the numerical implementation of PyBaMM improves. Regarding accuracy, the method overestimates the electrolyte depletion at 248 K and 2C discharge, driving the electrolyte concentration below the P2D value and ending the discharge about 100 s earlier than the P2D model. In contrast, the errors are smaller in charging, where the cell reaches the cut-off voltage before the electrolyte depletion builds up, with a voltage RMSE of about 11 mV at 1C. Under driving profiles, as shown in Fig. 6, the SPMe of this study remains stable and keeps a voltage RMSE of about 3.1 mV even for the UDSS profile.

3.4. Limitations of the present method

This section identifies the operating range where the proposed method is accurate and where its accuracy degrades. Under harsher conditions, the reaction current density becomes more non-uniform across the electrode while the proposed method assumes uniform current density. Therefore, the difference between the P2D and the SPMe increases with thicker electrodes, higher C-rate, and lower temperatures.

Fig. 8 presents the constant-current discharge curves from 298 K to 248 K with varying electrode thicknesses. The voltage RMSE for C-rate, temperature, and electrode thickness is reported in Fig. S9. For the case with the base electrode thickness, the method stays accurate at all C-rates down to 273 K. At 298 K, the voltage RMSE becomes noticeable for the case with 2× electrode thickness at 4C discharge (Fig. 8a–c). At 273 K, the 2C discharge stays accurate for the base thickness with a voltage RMSE of 1.58 mV, while it ends about 130 s early for electrodes with 1.5 times the baseline thickness and about 240 s early for electrodes with twice the baseline thickness (Fig. 8d–f). At 248 K, the 1C discharge stays accurate for the base thickness with a voltage RMSE of 3.83 mV, while it ends about 600 s early at 1.5× thickness and about 150 s early at 2× thickness (Fig. 8g–i).

In contrast, the driving profiles stay accurate for all thicknesses and temperatures. Fig. 8j–l presents the voltage RMSE under the FUDS profile for the three thicknesses at each temperature. The RMSE grows as the electrode becomes thicker and the temperature decreases, but the largest value is only 3.95 mV for the 2 times thicker electrode at 248 K. Charge and discharge alternate in a driving profile, and the current does not flow in one direction long enough for the electrolyte depletion to

accumulate. In EVs, the instantaneous current can be high, but the average over a full drive is only about 0.3 to 0.4C. The SPMe of this study therefore remains suitable for electric-vehicle analysis, even for a thick electrode at very low temperature (Fig. 8j–l and S8). The SPMe of this study is not a suitable choice for thick electrodes and cold temperatures with constant current input, while this SPMe can be a useful choice for simulating driving profiles at a wide range of temperatures.

4. Conclusions

Lithium-ion battery models have evolved from the P2D model to reduced-order models such as SPM and SPMe over the past decades [33, 40, 43]. While these reduced models have been developed to address computational challenges, a trade-off between voltage prediction accuracy and computational time has remained [47, 48].

We proposed a non-iterative method that solves the governing equations of the SPMe sequentially. We showed that SPMe can be solved non-iteratively if classical numerical techniques are arranged in the right order. Considering that electrolyte transport properties change relatively slowly with time, the method keeps concentration- and temperature-dependent electrolyte properties within this non-iterative structure by obtaining them in an explicit manner. We also applied the effective diffusion length for obtaining the coefficient for the FVM-based 3-by-3 matrices describing the electrolyte transport.

The proposed method was validated against the P2D model and compared with the PyBaMM SPMe under constant-current and driving profiles from 248 to 298 K. In terms of total computation time, it solves a constant-current discharge in about 0.1 ms and a driving profile in about 1 to 2 ms. Based on the total computation time, 10,000 simulations finish in about 1 s for constant current and in about 10 to 20 s for driving profiles. The voltage RMSE against the P2D model stays within about 5 mV for constant-current operation at 273 K and above, and within about 4 mV for driving profiles even at 248 K. The accuracy degrades in constant-current discharge at low temperature, high C-rate, and thick electrodes, where the electrolyte depletion is overestimated under the uniform reaction current assumption. For these conditions, the P2D model is the appropriate choice.

Within its validated range, the computational efficiency and accuracy of the SPMe solved using the proposed method make it well suited to simulation-intensive applications such as parameter identification [38, 50], multi-scale simulations [64–66], and the design of safe and fast charging protocols [67–70]. Future work is ongoing to extend the present SPMe to two-phase LFP electrodes [71, 72], mechanical deformation in graphite/silicon composite anodes [73], and degradation mechanisms [14–16].

CRedit authorship contribution statement

Soomin Choi: Writing – review & editing, Writing – original draft, Validation, Software, Formal analysis. **Minseo Kim:** Visualization, Validation, Software, Formal analysis, Data curation. **Susheel Teja Gogineni:** Writing – original draft, Supervision. **Jinyong Kim:** Writing – review & editing, Writing – original draft, Supervision, Software, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jpowsour.2026.241369>.

Nomenclature

List of symbols	
a_s	Specific active surface area for active materials [m^{-1}]
a_c, a_w, a_e, b	FVM coefficients for center, west, east, and right-hand side source term
c_e	Electrolyte concentration [$mol\ m^{-3}$]
c_s	Concentration of Li+ in active materials [$mol\ m^{-3}$]
$c_{s,surf}$	Concentration of Li+ at the surface of active materials [$mol\ m^{-3}$]
$c_{s,max}$	Maximum solid-phase lithium concentration [$mol\ m^{-3}$]
$A_{k\pm 1/2}$	Interface area at west/east face of node k [m^2]
$A_{neg/sep}, A_{sep/pos}$	Interface areas between adjacent regions [m^2]
D_s^{eff}	Effective diffusivity of Li+ in active materials [$m^2\ s^{-1}$]
D_e^{eff}	Effective electrolyte diffusivity [$m^2\ s^{-1}$]
I_{app}	Applied current density [$A\ m^{-2}$]
j^{Li}	Volumetric current density for the electrochemical reaction [$A\ m^{-3}$]
k_0	Rate constant for the electrochemical reaction at 298 K [$m^{2.5}\ mol^{-0.5}\ s^{-1}$]
k	Rate constant for the electrochemical reaction [$m^{2.5}\ mol^{-0.5}\ s^{-1}$]
R_{film}	Surface film resistance [$\Omega\ m^2$]
U_{eq}	Equilibrium potential [V]
$L_{neg}, L_{sep}, L_{pos}$	Thicknesses of negative electrode, separator, and positive electrode [m]
R_s	Particle radius [m]
ΔV	Control volume [m^3]
Δx	Node-to-interface distance in x-direction [m]
Δr	Radial node-to-interface distance [m]
Greek	
ε_e	Electrolyte volume fraction (porosity) [–]
ε_s	Volume fraction of the solid active material [–]
ϕ_e	Electrolyte potential [V]
ϕ_s	Electrode potential [V]
σ_s^{eff}	Effective electrical conductivity in the electrode [$S\ m^{-1}$]
κ^{eff}	Effective electrolyte conductivity [$S\ m^{-1}$]
κ_D^{eff}	Effective diffusional conductivity [$S\ m^{-1}$]
Superscripts and Subscripts	
neg	Negative electrode
sep	Separator
pos	Positive electrode
—	Spatially averaged (volume-averaged) quantity over the control volume
$(\cdot)^0$	Value at the previous time step
0	Initial value

Data availability

Data will be made available on request.

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