

Short communication

Comparison of approximate solution methods for the solid phase diffusion equation in a porous electrode model

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Abstract

Approximation methods are often used in porous electrode models to eliminate the need to solve the local solid phase diffusion equation. These methods include Duhamel's superposition method, a diffusion length method and a polynomial approximation method which have long been used in the literature. The pseudo steady state (PSS) method is a method that has been used recently to develop a solution to the diffusion equation in a spherical particle with time dependent boundary conditions, but the PSS method has not been used in a porous electrode model. These methods are compared to each other in a dimensionless analysis study, and they are used in a porous electrode model to predict the discharge curves for a LiCoO₂ electrode. Simulation results presented here indicate that the PSS method or the high order polynomial method should be used in a porous electrode model to obtain accuracy and save computation time.

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1. Introduction

Porous electrode models have been used widely to study the cell performance of various lithium based battery systems [1–8]. These models include mass transport in the liquid phase, electronic conduction in the solid phase and liquid phase in macro-scale and lithium diffusion inside solid phase particles at a local position in the porous electrode. The lithium transport in the solid phase is usually described by Fick's second law for a spherical particle:

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

$$-D_s \frac{\partial c_s}{\partial r} \Big|_{r=0} = 0 \quad (1b)$$

$$-D_s \frac{\partial c_s}{\partial r} \Big|_{r=R_s} = j_n \quad (1c)$$

The porous electrode model solution requires solving this particle diffusion equation in the an extra pseudo-dimension r . Consequently, the number of unknown variables in the model is much larger, which requires more computation time. Therefore, approximation methods are often used in porous electrode models to eliminate the need for the time consuming calculation of solid phase diffusion in the extra r dimension. These methods include a Duhamel's superposition method [1,2], a diffusion length method [9,10] and a polynomial approximation method [11,12]. In addition, Liu [13] developed recently an analytical solution to the diffusion problem with time dependent boundary conditions based on Ölçer's pseudo steady state (PSS) approach [14,15]. To our knowledge, Liu's method has not yet been used a porous electrode model. In this work, these approximation methods are compared to each other in a dimensionless analysis study, and they are used in a porous electrode model to simulate the discharge profiles of a LiCoO₂ electrode. The advantages and disadvantages of these methods are discussed based on the results from both studies. This work provides useful information to help one choose an approximation method for his specific application to maintain accuracy and save computation time.

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Nomenclature

Brug	Bruggeman coefficient
c_{\max}	maximum Li^+ concentration in the particles (mol cm^{-3})
c_s	Li^+ concentration in the solid particles (mol cm^{-3})
\bar{c}_s	volume averaged Li^+ concentration inside spherical particles (mol cm^{-3})
c_{se}	Li^+ concentration at the surface of the solid particles (mol cm^{-3})
C	dimensionless Li^+ concentration
D_e	diffusion coefficient of the electrolyte ($\text{cm}^2 \text{s}^{-1}$)
D_s	solid phase Li^+ diffusion coefficient in the particles ($\text{cm}^2 \text{s}^{-1}$)
f_{\pm}	mean molar salt activity coefficient
F	Faraday's constant ($96,487 \text{ C mol}^{-1}$)
j_n	pore wall flux ($\text{mol}(\text{cm}^2 \text{s})^{-1}$)
k	summation counter in Eq. (2b) represents previous time steps
k_p	kinetic rate constant ($(\text{mol}(\text{cm}^2 \text{s})^{-1})(\text{mol cm}^{-3})^{-1.5}$)
l_s	diffusion length of a spherical particle (cm)
n	summation counter in Eq. (2b) represents current time step
q_m	summation term used in (Eq. (9c))
\bar{q}_i	volume averaged concentration flux (mol cm^{-4})
R	gas constant ($8.3145 \text{ J}(\text{mol K})^{-1}$)
R_s	radius of the spherical particles (cm)
R_f	contact resistance ($\Omega \text{ cm}^2$)
S	geometric area of the electrode (cm^2)
t	time (s)
t_+^0	transference number of the electrolyte
T	temperature (K)
U_{eq}	equilibrium potential of the electrode (V)
v	thermodynamic factor of the electrolyte
W	active material loading in the electrode (g)
x	dimensionless distance in spherical particles

Greek letters

α_a, α_c	transfer coefficients
β	symmetry factor
δ	dimensionless pore wall flux
δ_p, δ_s	electrode or separator thickness (cm)
$\varepsilon_e, \varepsilon_s$	volume fraction of the electrolyte or active material in solid phase
ϕ_e, ϕ_s	liquid or solid phase potential (V)
κ_e	conductivity of the electrolyte (S cm^{-1})
λ_m	positive eigen-value determined from Eq. (9d)
σ_s	conductivity of the solid phase (S cm^{-1})
τ	dimensionless time

2. Overview on approximation methods**2.1. Duhamel's superposition method**

Duhamel's superposition method was the first approximation method [1,2] used in the porous electrode model. Duhamel's method relates the solution of a boundary value problem with time dependent boundary conditions to the solution of a similar problem with time-independent boundary conditions by means of a simple relation [16]. The Duhamel superposition equation for the solid phase diffusion equation is [1,2]:

$$\frac{D_s}{R_s} \frac{\partial c_s}{\partial r} \Big|_{r=R_s} = \sum_{k=0}^{n-2} \frac{(c_{s,k+1} - c_{s,k})}{\Delta t} A_{n-k} + \frac{(c_{s,n} - c_{s,n-1})}{\Delta t} A_1 \quad (2a)$$

where

$$A_{n-k} = a[(n-k)\Delta t] - a[(n-k-1)\Delta t] \quad (2b)$$

and

$$a(t) = \int_0^t \frac{\partial \bar{c}_s}{\partial r}(R_s, \zeta) d\zeta \quad (2c)$$

An expression for $a(t)$ was developed by using the Laplace transformation technique for short times and long times [1,2] and can be written in terms of a dimensionless time $\tau = tD_s/R_s^2$:

$$a(\tau) = -\tau + 2\left(\frac{\tau}{\pi}\right)^{1/2} \left[1 + 2 \sum_{n=1}^{\infty} \left(\exp\left(\frac{-n^2}{\tau}\right) - n\left(\frac{\pi}{\tau}\right)^{1/2} \operatorname{erfc}\left(\frac{n}{\sqrt{\tau}}\right) \right) \right] \quad \text{short time} \quad (3a)$$

$$a(\tau) = \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} [1 - \exp(-n^2\pi^2\tau)] \quad \text{long time} \quad (3b)$$

The expressions (Eqs. (3a) and (3b)) are both uniformly valid. However, Eq. (3a) converges more quickly with fewer terms at short times than Eq. (3b).

The relation between the surface concentration at current time step $c_{s,n}$ and time dependent pore wall flux j_n can be established through Eqs. (1c) and (2a) as follow:

$$-\frac{j_n}{R_s} = \sum_{k=0}^{n-2} \frac{(c_{s,k+1} - c_{s,k})}{\Delta t} A_{n-k} + \frac{(c_{s,n} - c_{s,n-1})}{\Delta t} A_1 \quad (4a)$$

It should be noted that values of the surface concentration from all previous time steps $c_{s,k}$ are required in Eq. (4a) to calculate the value at current time step $c_{s,n}$. The volume averaged concentration \bar{c}_s in the spherical particles can be readily calculated as follow:

$$\bar{c}_s = c_0 + \int_0^t -\frac{3}{R_s} j_n dt \quad (4b)$$

2.2. Diffusion length method

Wang et al. [9] used diffusion length concept to simplify the solid phase diffusion equation in the porous electrode model. By

assuming a parabolic concentration profile in the diffusion layer and using the volume average technique, they determined the diffusion length to be $R_s/5$ for spherical particles. The solution of Eqs. (1a)–(1c) can be approximated with a set of differential and algebraic equations:

$$\frac{\partial \bar{c}_s}{\partial t} = -\frac{3}{R_s} j_n \quad (5a)$$

$$\frac{D_s}{l_s} (c_{se} - \bar{c}_s) = -j_n \quad (5b)$$

where l_s is the diffusion length and takes the value of $R_s/5$ for spherical particles.

The diffusion length method predicts that the surface concentration and volume averaged concentration inside a particle are linearly dependent on each other, which should be valid only after the diffusion layer builds up to its steady state. Therefore, the method is inadequate at short times or under dynamic operations, such as pulse or current interrupt operations.

In view of the shortcoming of the diffusion length method, Wang and Srinivasan [10] corrected the diffusion length method by empirically incorporating an intuitively expressed time dependent term into the diffusion length equations:

$$\frac{\partial \bar{c}_s}{\partial t} = -\frac{3}{R_s} j_n \quad (6a)$$

$$\frac{D_s}{l_s} (c_{se} - \bar{c}_s) = -j_n \left(1 - \exp\left(-\frac{4}{3} \frac{\sqrt{D_s t}}{l_s}\right) \right) \quad (6b)$$

The empirical term was formed based on the observation that the surface concentration increases exponentially at short times. The value of the multiplier in the exponential term was determined by matching the surface concentration profiles obtained with Eqs. (6a) and (6b) at given pore wall fluxes to those from Duhamel's method. The value of $4/3$ was found to be able to provide good results under a wide range of operating conditions [10].

2.3. Polynomial approximation method

Polynomial approximation method [11,12] by Subramanian et al. (see also Rice and Do [17], Chapter 12) was also based on the parabolic concentration profile assumption and volume averaging technique. The authors first assumed that the concentration profile could be described by a second order polynomial ($c = a + br^2$) and the equations for low order polynomial method were derived as:

$$\frac{\partial \bar{c}_s}{\partial t} = -\frac{3}{R_s} j_n \quad (7a)$$

$$\frac{5D_s}{R_s} (c_{se} - \bar{c}_s) = -j_n \quad (7b)$$

To achieve better accuracy at short times, the authors [11,12] used a higher order polynomial ($c = a + br^2 + dr^4$) model for the concentration profile. The equations for this high order polynomial method are as follows:

$$\frac{\partial \bar{c}_s}{\partial t} = -\frac{3}{R_s} j_n \quad (8a)$$

$$\frac{d\bar{q}_t}{dt} + 30 \frac{D_s}{R_s^2} \bar{q}_t + \frac{45}{2} \frac{j_n}{R_s^2} = 0 \quad (8b)$$

$$\frac{35D_s}{R_s} (c_{se} - \bar{c}_s) - 8D_s \bar{q}_t = -j_n \quad (8c)$$

where \bar{q}_t is the volume averaged concentration flux which physically defines the change of concentration with respect to the position in the system [12].

This high order polynomial method uses a different approach from the diffusion length method to improve the solution accuracy at short times. The diffusion length method uses the empirical exponential term in the equation and determines the multiplier value by matching surface concentration profiles to the exact solutions. The high order polynomial method uses a higher order polynomial for the concentration profile in the derivation, and one could derive new sets of equations with an even higher order polynomial model, if needed, following the same procedures discussed in the papers [11,12].

2.4. Pseudo steady state method

Liu [13] applied Ölçer's pseudo steady state (PSS) method [14,15], which is a form of a finite integral transform technique to eliminate the independent spatial variable r from the solid phase diffusion equation. For diffusion problems with a time dependent pore wall flux j_n as a boundary condition described by Eqs. (1a)–(1c), the generalized PSS solution was found to be [13]:

$$\frac{\partial \bar{c}_s}{\partial t} = -\frac{3}{R_s} j_n \quad (9a)$$

$$\frac{\partial q_m}{\partial t} = \frac{\lambda_m^2 D_s}{R_s^2} e^{\lambda_m^2 D_s t / R_s^2} j_n \quad (9b)$$

$$c_{se} - \bar{c}_s = -\frac{R_s}{5D_s} j_n + \frac{2R_s}{D_s} \sum_{m=1}^{\infty} \frac{\sqrt{1 + \lambda_m^2}}{\lambda_m^2} (-1)^m \sin(\lambda_m) \times [j_n - e^{-\lambda_m^2 D_s t / R_s^2} q_m] \quad (9c)$$

where q_m is denoted only as a summation term in Eq. (9c) and itself does not have a physical meaning. The λ_m values were determined from the eigenvalue equation:

$$\lambda_m = \tan(\lambda_m) \quad (9d)$$

Eqs. (9a)–(9d) were developed and implemented only for diffusion in spherical particles. However, the PSS method could be extended to diffusion in particles with other geometries, such as disks and cylinders, following the procedures detailed in the Ref. [13].

3. Dimensionless analysis

Before these approximation methods are used in a porous electrode model, we use dimensionless analysis to compare how these methods perform on diffusion problems with time dependent boundary conditions. Eqs. (1a)–(1c) are converted to

dimensionless form using following dimensionless variables:

$$C = \frac{c_s}{c_{\max}}, \quad x = \frac{r}{R_s}, \quad \tau = \frac{D_s t}{R_s^2}, \quad \delta(\tau) = \frac{j_n R_s}{D_s c_{\max}} \tag{10}$$

The governing equation and boundary conditions in dimensionless forms are:

$$\frac{\partial C}{\partial \tau} = \frac{1}{x^2} \left(x^2 \frac{\partial C}{\partial x} \right) \tag{11a}$$

$$\left. \frac{\partial C}{\partial x} \right|_{x=0} = 0 \tag{11b}$$

$$\left. \frac{\partial C}{\partial x} \right|_{x=1} = -\delta(\tau) \tag{11c}$$

The exact solutions to the dimensionless diffusion equations are compared to those obtained from approximation methods in Figs. 1 and 2 where the dimensionless surface concentration minus the volume averaged concentration is plotted against dimensionless time. The dimensionless pore wall flux $\delta(\tau)$ takes the form of $1 - \tau$ and $\sin(5\tau)$, respectively, in the figures. The finite difference method with 100 internal node points was used to find a numerical solution to Eqs. (11a)–(11c) and is named the exact solution. Two summation terms are used in PSS method (m equal to 2).

As shown in Figs. 1 and 2, the low order polynomial method (or uncorrected diffusion length method) is inadequate at short times for transient behavior. The method fails to converge to the exact solution at steady state. Further simulation shows that the solution of low order polynomial method will match the exact solution at long times only when the pore wall flux j_n or $\delta(\tau)$ is a constant. Although the corrected diffusion length method provides improved accuracy at short times by incorporating the empirical exponential term, it has the same problem as the uncorrected method at long times where the exponential term becomes close to zero (see Eqs. (6a) and (6b)). These simulation results

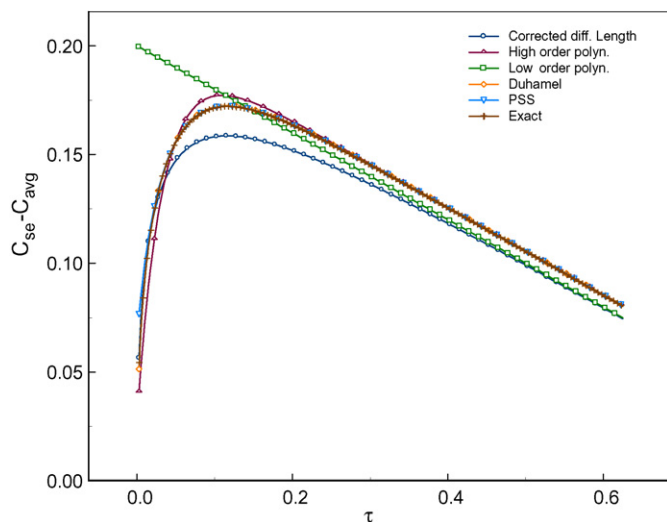


Fig. 1. Comparison of approximation solutions with the exact solution of the dimensionless diffusion equation. $\delta(\tau) = 1 - \tau$.

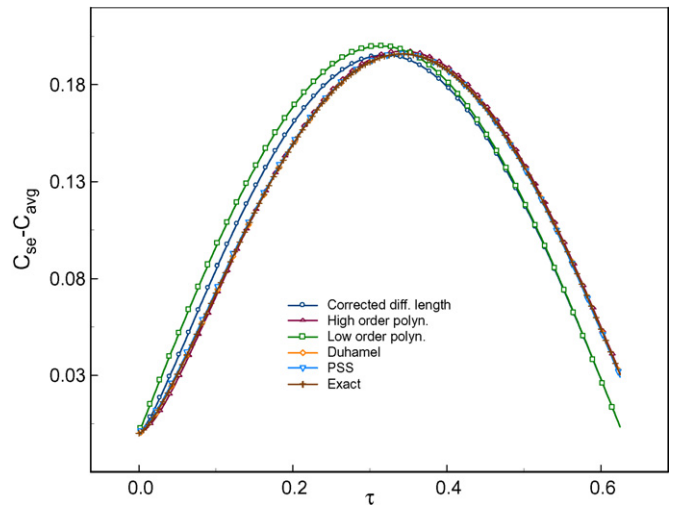


Fig. 2. Comparison of approximation solutions with the exact solution of the dimensionless diffusion equation. $\delta(\tau) = \sin(5\tau)$.

indicate that the low order polynomial method and the corrected diffusion length method cannot provide as accurate results as the Duhamel’s superposition method, the PSS method or the high order polynomial method.

By using a high order polynomial model for the concentration profile in the solid particles, the high order polynomial method is not only able to describe transient behavior in more detail, but also it is able to provide much more accurate results at long times. In addition, the method remains computational simplistic and can be easily implemented in a porous electrode model.

The usage of the PSS method is mainly affected by the number of summation terms included. If no summation terms are used, the method degrades to the low order polynomial method. Increasing the number of summation terms improves the accuracy of the method, mostly at short times. Our simulation shows that PSS method with two or three summation terms is able to provide accurate results under a wide range of operating conditions. More summation terms require solving more differential equations (Eq. (9b)) and could pose numerical difficulties because of the exponential terms. Fig. 3 shows that the PSS method with four summation terms must be solved with a tightened error tolerance in order to obtain accurate results when the dimensionless pore wall flux is $\delta(\tau) = \sin(5\tau)$. If the PSS method is used in the porous electrode model, the approximation equations are tightly coupled to other equations for the liquid phase concentration and potentials. The smaller error tolerance required by the PSS method with several summation terms could have negative effects on solving the whole equation system, rendering it computationally more intensive.

The Duhamel’s superposition method can provide the most accurate solutions when used with a small time step Δt . However, this also leads to its disadvantages. The method requires significantly more computation time when the time frame is long and the time step is small. It also demands more storage space to record values of dependent variables from all previous time steps because those values are required in the calculation for the current time step (Eq. (2a)). When the method is used in porous

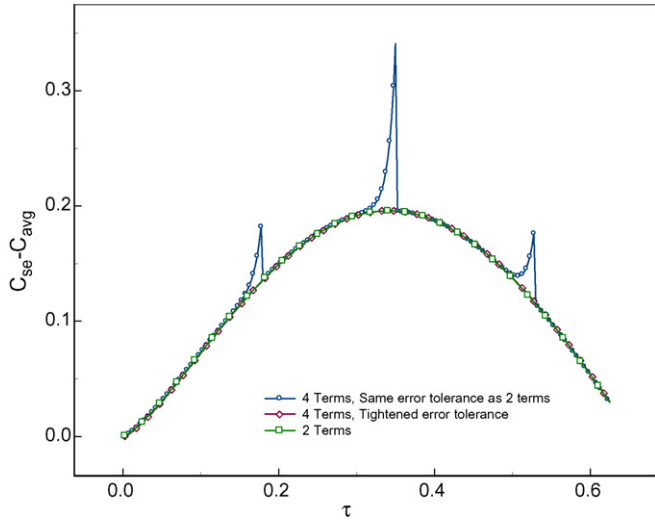


Fig. 3. A tight error tolerance is required to solve PSS method with more summation terms. PSS method with four summation terms requires smaller error tolerance to get accurate results. $\delta(\tau) = \sin(5\tau)$.

electrode model and localized at each discretization node along spatial coordinates, the computation and storage requirement become exacerbated, as will be shown in the following section.

The preliminary dimensionless analysis indicates that pseudo steady state method and the high order polynomial method would be good choices for the use in porous electrode model. In the following, we will compare the usage of the approximation methods in a porous electrode model to predict discharge profiles of a LiCoO_2 half cell.

4. Approximation methods in a porous electrode model

Equations for a porous electrode model have been described extensively in many papers [1,2] and they will not be repeated here. The discharge profiles of a LiCoO_2 electrode were measured in an experiment, the details of which were revealed elsewhere [18]. A pseudo-2D porous electrode model was used in the study to simulate the discharge profiles. By pseudo-2D, we mean that the model is solved in the spatial coordinate x along with the solid phase diffusion equation being solved in the extra r dimension at each x . In order to obtain good simulation results, the symmetry factor β in the Butler Volmer equation was empirically assumed to change with the cell state of discharge [18]. The empirical expression for the Butler Volmer equation was formulated as follows:

$$j_n = k_p c_e^{\alpha_a} (c_{\max} - c_{se})^{\alpha_a} c_{se}^{\alpha_c} \left(\exp \left(\frac{\alpha_a F}{RT} (\phi_s - \phi_e - U_{eq} - j_n FR_f) \right) - \exp \left(- \frac{\alpha_c F}{RT} (\phi_s - \phi_e - U_{eq} - j_n FR_f) \right) \right) \quad (12a)$$

$$\alpha_c = \beta = 0.5 \left(1 - \frac{1}{1 + \exp(a(b - c_{se}/c_{\max}))} \right) \quad (12b)$$

$$\alpha_a = 1 - \beta \quad (12c)$$

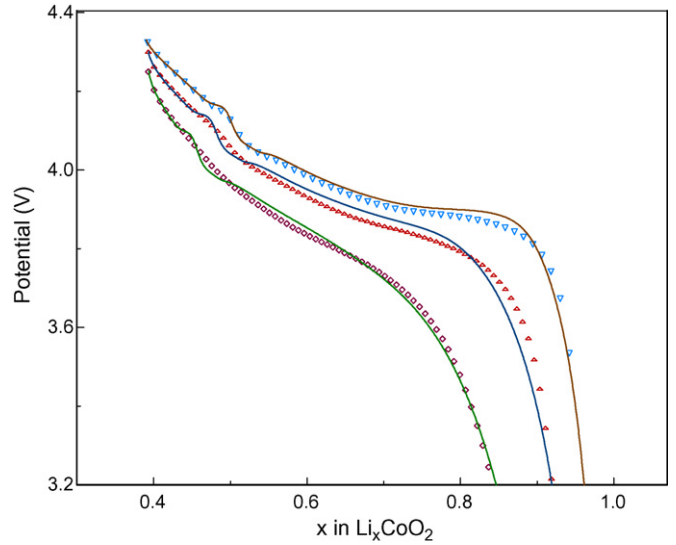


Fig. 4. Experimental (symbols) and simulated (lines) discharge profiles at different current rates. The rates from top to bottom: $C/7$, $C/2.7$, and $C/1.3$ ($C = 4 \text{ mA}$). The pseudo-2D porous electrode model well captures the effect of increased solid phase diffusion limitation at higher current rates indicated by the increased curvature at the beginning of discharge.

Fig. 4 presents a comparison of the experimental and simulated discharge profiles using the pseudo-2D porous electrode model at different current rates: $C/7$, $C/2.7$, and $C/1.3$ ($C = 4 \text{ mA}$). The pseudo-2D model captures well the effect of increased solid phase diffusion limitation at higher current rates, as indicated by the increased curvature at the beginning of discharge profiles. The parameters used in the simulation are listed in Table 1.

The approximation methods are used next in the porous electrode model to eliminate the need to solve the solid phase diffusion equation in the r direction. These models use the same parameters given in Table 1 and the simulation results are compared with those obtained using the pseudo-2D model in Figs. 5–7.

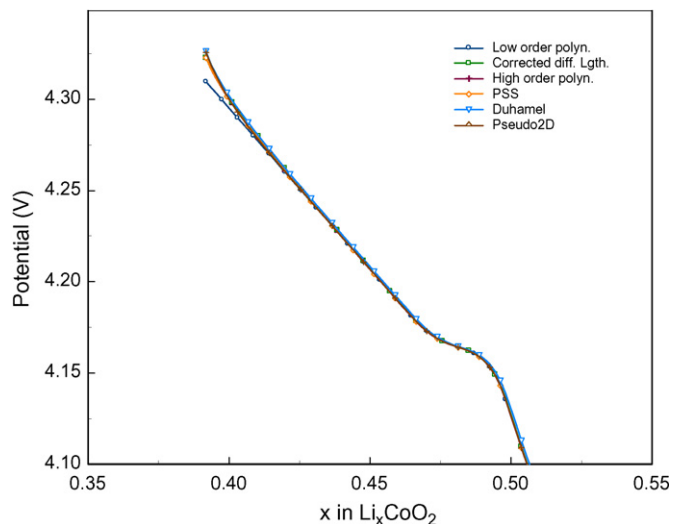


Fig. 5. Comparison of simulation results from porous electrode models with approximation methods and pseudo-2D model. Discharge rate is $C/7$ ($C = 4 \text{ mA}$).

Table 1
Model parameters used to simulate the discharge curves

Parameter	Value
LiCoO₂ electrode	
T (°C)	15 ^a
W (g)	0.0245 ^a
δ_p (cm)	64×10^{-4a}
ϵ_e	0.30 ^a
S (cm ²)	1.267 ^a
R_s (cm)	10×10^{-4a}
σ_s (S cm ⁻¹)	0.1 ^b
Brug	1.5 ^b
D_s (cm ² s ⁻¹)	1.2×10^{-10c}
R_f (Ω cm ²)	200 ^c
$x_{0,p}$	0.393 ^c
k_p	2.59×10^{-6c}
Separator	
$c_{e,0}$	1×10^{-3a}
δ_s (cm)	25×10^{-4a}
$\log(D_e)$ (cm ² s ⁻¹)	$-4.43 - 54/(T - 5 \times 10^3 c_e - 229) - 0.22 \times 10^3 c_e^d$
κ_e (S cm ⁻¹)	$c_e(-10.5 + 0.074T - 6.96 \times 10^{-5}T^2 + 668c_e - 17.8c_eT + 0.028c_eT^2 + 4.94 \times 10^5c_e^2 - 886c_e^2T)^2d$
$v = (1 - t_+^0) \left(1 + \frac{d \ln f_{\pm}}{d \ln c_e}\right)$	$0.601 - 7.59c_e^{0.5} + 3.1 \times 10^4(2.53 - 0.0052T)c_e^{1.5d}$
S (cm ²)	1.267 ^a
ϵ_e	0.46 ^a
Parameters used in Eqs. (12a)–(12c)	
	a^c
	b^c
$C/7$	21
$C/2.7$	13
$C/1.3$	8

^a Manufacturer data or experiment data.
^b From Refs. [3,19,20].
^c Values fit to experiment data.
^d From Ref. [21].

The simulation results show that the choice of an approximation method is more important at high current rates than it is at low current rates. The long time behavior is also less affected than the short time behavior. The short time behavior is very

important in studying the discharge profiles of the LiCoO₂ electrode because it reflects valuable information about how severe the solid diffusion limitation is in the LiCoO₂ electrode. Simulation results obtained from the model using the low order

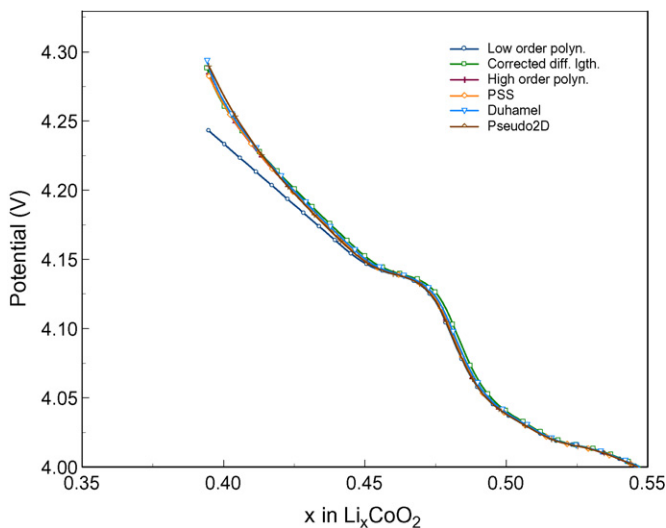


Fig. 6. Comparison of simulation results from porous electrode models with approximation methods and pseudo-2D model. Discharge rate is C/2.7 (C = 4 mA).

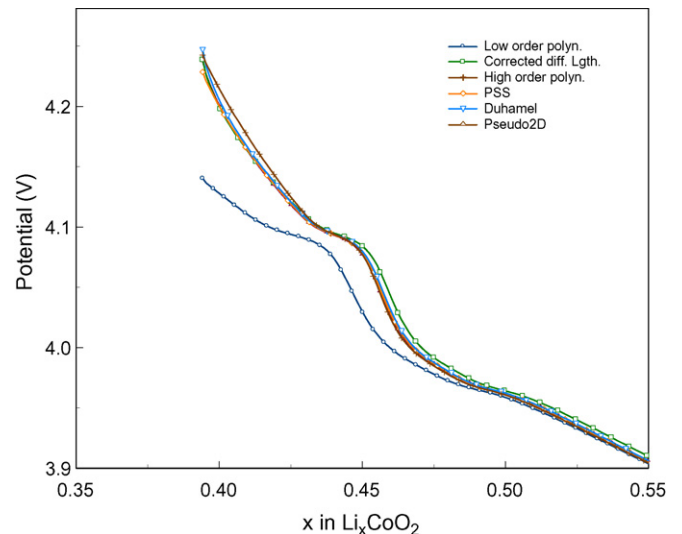


Fig. 7. Comparison of simulation results from porous electrode models with approximation methods and pseudo-2D model. Discharge rate is C/1.3 (C = 4 mA).

Table 2
Computation time (in seconds) required to solve the porous electrode models^a

	C/7	C/2.7	C/1.3
Low order polynomial	1	0.9	0.9
Corrected diffusion length	1.1	1.0	1.0
High order polynomial	1.2	1.1	1.1
Duhamel	62	89	87
PSS	1.5	1.4	1.3
Pseudo-2D	10.5	10	9.6

^a Average of five runs.

polynomial method (or uncorrected diffusion length method) have significant errors at the beginning of discharge, especially when the discharge current is high. The model basically failed to show how the solid phase diffusion influences the discharge curves of the LiCoO₂ electrode. The corrected diffusion length method provides significantly improved results compared to the uncorrected method in describing transient behaviors, but it tends to slightly over predict the cell potential. The model using the Duhamel superposition method is accurate, but it requires much more computation time than the pseudo-2D model. All other models using an approximation method have significant speed advantages over the pseudo-2D model. Table 2 lists the computation times required to solve these models using DASSL [22] solver. The model using the high order polynomial method provides good results at most times, but it is inferior to the PSS method at short times when the current is high. The PSS method stands out in the comparison because the model using the PSS method is able to provide simulation results not only with accuracy but also with a speed advantage. It should be noted that even though the study is based on a LiCoO₂ electrode with characteristic particles size of 10×10^{-4} cm, the models are expected to perform mostly the same as long as the lithium transport in the particles can be mathematically described through Fick's diffusion law (Eqs. (1a)–(1c)), regardless of the electrode materials and particle sizes.

5. Summary

Approximation methods are often used in porous electrode models to make them more computationally efficient. In this work, the Duhamel's superposition method, the corrected diffusion length method, the polynomial approximation method, and

the pseudo steady state method are compared to each other in a dimensionless analysis study, and they are used in a porous electrode model to describe the discharge profiles of a LiCoO₂ electrode in a half cell. The low order polynomial method was found to be inadequate for transient behavior in both studies. Although the corrected diffusion length method proved reasonably accurate at short times, this method did not converge to the exact solution at steady state. The Duhamel's superposition method requires extensive computation time and storage space. Simulation results show that porous electrode model using Duhamel's method requires even more computation time than the pseudo-2D model when the DASSL solver is used. This study indicates that the pseudo steady state method or the high order polynomial method should be considered first if an approximation method is to be used in a porous electrode model.

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