

A quick and efficient method for consistent initialization of battery models

Vijayasekaran Boovaragavan, Venkat R. Subramanian *

Department of Chemical Engineering, Tennessee Technological University, Cookeville, TN 38505, USA

Received 2 March 2007; received in revised form 6 April 2007; accepted 11 April 2007

Available online 21 April 2007

Abstract

Secondary batteries are usually modeled as a system of coupled nonlinear partial differential equations. These models are typically solved by applying finite differences or other discretization techniques in the spatial directions and solving the resulting system of differential algebraic equations (DAEs) numerically in time. These DAEs are very difficult to solve even using popular DAE solvers. The complications arise partly due to the difficulty in obtaining consistent, or closely consistent, initial conditions for the DAEs. In this paper, a shooting method is proposed as an effective and rapid technique for the initialization of battery models. This method is built on a region-wise shooting approach with initial guess at one end of the electrode and physics based shooting criterion on the other end that can ultimately satisfy all the required conditions in a battery unit. Notably, the computation time required for the proposed method is only milliseconds in a FORTRAN environment for the case of initializing a standard physics based lithium-ion battery model. Also the initial values obtained are exact and can readily be fed into any DAE solver for achieving accurate solutions without solver failure. This rapid method will help in simulating batteries in hybrid environments in real-time (milliseconds).

© 2007 Elsevier B.V. All rights reserved.

Keywords: Battery models; Differential–algebraic system; Shooting method

1. Introduction

Many investigations on electrochemical devices are focused on electric or hybrid vehicles in which lithium-ion battery chemistry plays a crucial role. A major problem encountered in electric or hybrid vehicles is the lack of on-board monitoring and control over the electrochemical components. This is due to the complexity in electrochemical models that makes their simulation very difficult, when compared to other models or time scale present in the hybrid system. The existing physics based electrochemical models are represented as a system of coupled nonlinear multiple partial differential equations (PDEs) in multiple domains that are usually written in differential–algebraic form for simulation and model analysis. To facilitate successful simulation of these models, there is a necessity for

an exact, consistent and rapid initialization of DAEs. Improper or heuristic initial values can lead to simulation failure even with popular DAE solvers like DASSL [1], GAMD [2], RADAU [3], *etc.* Sometimes approximate initialization may lead to quick solutions, but the solutions are not physically meaningful or inaccurate. Since the integration is started far away from the consistent initial values, the difference between approximate values and consistent values will contribute to a local error right from the very first step of integration. Some of the latest DAE solvers have features allowing a range for initializing each variable, but are unaffordable due to high computation time.

There are some specific techniques developed for the successful initialization of lithium-ion and other secondary battery models. Newman [4] has first started investigating this system by using an innovative BAND subroutine. Here, the initial conditions are obtained by solving the steady-state equations of the nonlinear DAE models using BAND. Zhang and Cheh [5] solved a similar model

* Corresponding author. Tel.: +1 931 372 3494; fax: +1 931 372 6352.
E-mail address: vsubramanian@tntech.edu (V.R. Subramanian).

Nomenclature

a_i	specific surface area of electrode i ($i = p, n$), m^2/m^3	R	universal gas constant, $\text{J}/(\text{mol K})$
brugg_i	Bruggman coefficient of region i ($i = p, s, n$)	R_i	radius of the intercalation particle of electrode i ($i = p, n$), m
c	electrolyte concentration, mol/m^3	s	separator
c_0	initial electrolyte concentration, mol/m^3	t_+	Li^+ transference number in the electrolyte
$c_{s,i}$	concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3	T	absolute temperature, K
$c_{s,i,0}$	initial concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3	U_i	open circuit potential of electrode i ($i = p, n$), V
$c_{s,i,\text{max}}$	maximum concentration of lithium ions in the intercalation particle of electrode i ($i = p, n$), mol/m^3	U_s	standard potential of the solvent reduction reaction, V
D	electrolyte diffusion coefficient, m^2/s	x	spatial coordinate, m
$D_{s,i}$	lithium-ion diffusion coefficient in the intercalation particle of electrode i ($i = p, n$), m^2/s	ε_i	porosity of region i ($i = p, s, n$)
F	Faraday's constant, C/mol	$\varepsilon_{f,i}$	volume fraction of fillers of electrode i ($i = p, n$)
I	applied current density, A/cm^2	θ_i	dimensionless concentration of lithium ions in the intercalation particle of electrode i ($\theta_i = c_{s,i}/c_{s,i,\text{max}}$)
j_i	wall flux of Li^+ on the intercalation particle of electrode i ($i = n, p$), mol/m^2	κ	ionic conductivity of the electrolyte, S/m
k_i	intercalation/deintercalation reaction rate constant of electrode i ($i = p, n$), $\text{mol}/(\text{mol}/\text{m}^3)^{1.5}$	$\kappa_{\text{eff},i}$	effective ionic conductivity of the electrolyte in region i ($i = p, s, n$), S/m
l_i	thickness of region i ($i = p, s, n$), m	σ_i	electronic conductivity of the solid-phase of electrode i ($i = p, n$), S/m
n	negative electrode	$\sigma_{\text{eff},i}$	effective electronic conductivity of the solid-phase of electrode i ($i = p, n$), S/m
p	positive electrode	Φ_1	solid-phase potential, V
r	radial coordinate, m	Φ_2	electrolyte phase potential, V

governing a Zn– MnO_2 system without using the traditional BAND technique. They used a HYBRID1 subroutine based on the Powell hybrid method that has provision to choose a tolerance limit. They claimed that it took less than 5% of the total time for solving the DAEs. Another initialization subroutine for DAE solvers called DAEIS was developed in the FORTRAN environment [6,7] based on the repeated solution of a set of nonlinear equations. The success of this method is based on the nonlinear equation solver used in the subroutine. This method has also been demonstrated for the model governing galvanostatic charge/discharge processes of a thin film nickel hydroxide electrode. Other rigorous methods developed for the initialization of general DAEs systems can be found in the literature [8,9].

Rigorous methods for the initialization of DAEs depend on the efficiency and robustness of nonlinear algebraic routines or optimization routines and may fail due to convergence problems. Moreover, they require more computation time, and hence are not ideal for applications such as parameter estimation, capacity fade analysis, on-board simulation and real-time optimization where repetitive simulation of DAEs are essential. Hence a simple, rapid and more robust method for DAEs initialization is of considerable interest.

The purpose of this paper is to introduce a novel and efficient method for initialization of DAEs experienced in

advanced battery models. This simple and effective initialization technique is based on the physical constraints imposed by the battery chemistry and the shooting method to meet these constraints using steady-state model equations. The method has been described and also demonstrated using a lithium-ion battery model in FORTRAN, Matlab® and Maple® environments. The proposed method can provide initial values quickly and consistently in any environments.

2. Proposed initialization method

The initial conditions for variables with time derivatives are set by the physical properties of the electrochemical system, only the variables without time derivatives are initialized. These equations are sometimes referred as

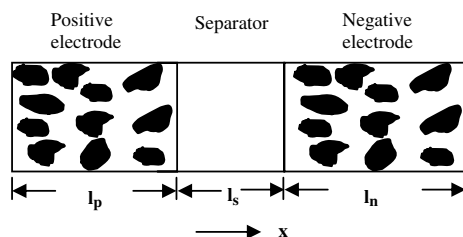


Fig. 1. Schematic representation of different regions in a lithium-ion cell.

Table 1
Pseudo-two-dimensional model for lithium-ion battery with boundary and initial conditions

Region	Governing equations	Boundary conditions
Positive electrode	$\varepsilon_p \frac{\partial c}{\partial t} = D_{\text{eff,p}} \frac{\partial^2 c}{\partial x^2} + a_p(1-t_+)j_p \text{ initial condition } c _{t=0} = c_0$ $-\sigma_{\text{eff,p}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\text{eff,p}}RT}{F}(1-t_+) \frac{\partial \ln c}{\partial x} = I$ $\sigma_{\text{eff,p}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_p F j_p$ $\frac{\partial c_s}{\partial t} = \frac{D_{s,p}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) \text{ initial condition } c_s _{t=0} = 0.5c_{s,\text{max,p}}$	$-D_{\text{eff,p}} \frac{\partial c}{\partial x} \Big _{x=0} = 0 \text{ and } -D_{\text{eff,p}} \frac{\partial c}{\partial x} \Big _{x=l_p,-} = -D_{\text{eff,s}} \frac{\partial c}{\partial x} \Big _{x=l_p,+}$ $-\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=0} = 0 \text{ and } -\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,-} = -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,+}$ $\frac{\partial \Phi_1}{\partial x} \Big _{x=0} = -\frac{I}{\sigma_{\text{eff,p}}} \text{ and } -\sigma_{\text{eff,p}} \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p} = 0$ $\frac{\partial c_s}{\partial r} \Big _{r=0} = 0 \text{ and } j_p = -D_{s,p} \frac{\partial c_s}{\partial r} \Big _{r=R_p}$
Separator	$\varepsilon_s \frac{\partial c}{\partial t} = D_{\text{eff,s}} \frac{\partial^2 c}{\partial x^2}$ $I = -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\text{eff,s}}RT}{F}(1-t_+) \frac{\partial \ln c}{\partial x}$	$-D_{\text{eff,p}} \frac{\partial c}{\partial x} \Big _{x=l_p,-} = -D_{\text{eff,s}} \frac{\partial c}{\partial x} \Big _{x=l_p,+} \text{ and } -D_{\text{eff,s}} \frac{\partial c}{\partial x} \Big _{x=l_p+l_s,-} = -D_{\text{eff,n}} \frac{\partial c}{\partial x} \Big _{x=l_p+l_s,+}$ $-\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,-} = -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,+} \text{ and } -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,-} = -\kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,+}$
Negative electrode	$\varepsilon_n \frac{\partial c}{\partial t} = D_{\text{eff,n}} \frac{\partial^2 c}{\partial x^2} + a_n(1-t_+)j_n \text{ initial condition } c _{t=0} = c_0$ $-\sigma_{\text{eff,n}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} + \frac{2\kappa_{\text{eff,n}}RT}{F}(1-t_+) \frac{\partial \ln c}{\partial x} = I$ $\sigma_{\text{eff,n}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_n F j_n$ $\frac{\partial c_s}{\partial t} = \frac{D_{s,n}}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) \text{ initial condition } c_s _{t=0} = 0.85c_{s,\text{max,n}}$	$-D_{\text{eff,s}} \frac{\partial c}{\partial x} \Big _{x=l_p+l_s,-} = -D_{\text{eff,n}} \frac{\partial c}{\partial x} \Big _{x=l_p+l_s,+} \text{ and } -D_{\text{eff,n}} \frac{\partial c}{\partial x} \Big _{x=l_p+l_s+l_n} = 0$ $-\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,-} = -\kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,+} \text{ and } \Phi_2 \Big _{x=l_p+l_s+l_n} = 0$ $-\sigma_{\text{eff,n}} \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p+l_s} = 0 \text{ and } \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p+l_s+l_n} = -\frac{I}{\sigma_{\text{eff,n}}}$ $\frac{\partial c_s}{\partial r} \Big _{r=0} = 0 \text{ and } j_n = -D_{s,n} \frac{\partial c_s}{\partial r} \Big _{r=R_n}$

Table 2
Steady-state model of lithium-ion battery used for evaluating initial values

Region	Governing equations	Boundary conditions
Positive electrode	$-\sigma_{\text{eff,p}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} = I$ $\sigma_{\text{eff,p}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_p F j_p$ $c_s _{r=R_p} = \frac{-j_p}{3(N+1)} \frac{R_p}{D_{s,p}} + c_{s,\text{max,p}}$	$-\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=0} = 0 \quad \text{and} \quad -\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,-} = -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,+}$ $\frac{\partial \Phi_1}{\partial x} \Big _{x=0} = -\frac{I}{\sigma_{\text{eff,p}}} \quad \text{and} \quad -\sigma_{\text{eff,p}} \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p} = 0$
Separator	$-\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} = I$	$-\kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,-} = -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p,+} \quad \text{and} \quad -\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,-} = -\kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,+}$
Negative electrode	$-\sigma_{\text{eff,n}} \frac{\partial \Phi_1}{\partial x} - \kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} = I$ $\sigma_{\text{eff,n}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_n F j_n$ $c_s _{r=R_p} = \frac{-j_n}{3(N+1)} \frac{R_p}{D_{s,n}} + c_{s,\text{max,n}}$	$-\kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,-} = -\kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} \Big _{x=l_p+l_s,+} \quad \text{and} \quad \Phi_2 \Big _{x=l_p+l_s+l_n} = 0$ $-\sigma_{\text{eff,n}} \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p+l_s} = 0 \quad \text{and} \quad \frac{\partial \Phi_1}{\partial x} \Big _{x=l_p+l_s+l_n} = -\frac{I}{\sigma_{\text{eff,n}}}$

$$j_p = 2k_p(c_{s,\text{max,p}} - c_s|_{r=R_p})^{0.5} c_s|_{r=R_p}^{0.5} c^{0.5} \sinh \left[\frac{0.5F}{RT} (\Phi_1 - \Phi_2 - U_p) \right] \quad \text{and} \quad j_n = 2k_n(c_{s,\text{max,n}} - c_s|_{r=R_p})^{0.5} c_s|_{r=R_p}^{0.5} c^{0.5} \sinh \left[\frac{0.5F}{RT} (\Phi_1 - \Phi_2 - U_n) \right],$$

$$U_p = \frac{-4.656+88.669\theta_p^2-401.119\theta_p^3+342.909\theta_p^4-462.471\theta_p^5+433.434\theta_p^{10}}{-1.0+18.933\theta_p^2-79.532\theta_p^3+37.311\theta_p^4-73.083\theta_p^5+95.960\theta_p^{10}}; \quad \theta_p = c_s|_{r=R_p}/c_{s,\text{max,p}},$$

$$U_n = 0.7222 + 0.1387\theta_n + 0.029\theta_n^{0.5} - \frac{0.0172}{\theta_n} + \frac{0.0019}{\theta_n^{1.5}} + 0.2808 \exp(0.90 - 15\theta_n) - 0.7984 \exp(0.4465\theta_n - 0.4108); \quad \theta_n = c_s|_{r=R_p}/c_{s,\text{max,n}}.$$

steady-state equations. The components of a secondary battery such as positive electrode, separator and negative electrode can be arranged as three regions as shown in Fig. 1. Since the separator consists of liquid electrolyte alone, the steady-state model governing this region is only a single ordinary differential equation (ODE) in x that can lead to a closed-form solution.

The lithium-ion battery model [4,10] used to demonstrate the proposed rapid initialization method is given in Table 1. This rigorous two-dimensional model consists of three independent variables (x , r and t) and four dependent variables (c , Φ_1 , Φ_2 , c_s). It has a total of ten coupled nonlinear PDEs that are to be solved simultaneously. A successful simulation of this model is possible only when the initial conditions are consistent, meaning that $f(t, x, x', r) = 0$. The steady-state form of these governing equations used for calculating the consistent initial values are given in Table 2. The solid-phase surface concentration is written in algebraic form using spatial discretization in the radial direction. This variable can also be represented in algebraic form using an efficient simplification method proposed by Subramanian et al. [10]. This has been tested for an entirely different set of model parameters [4]. The values of the parameters used in the simulation of model equations are given in Table 3 and Ref. [11]. The steps involved are given below:

1. Assume an initial value for unknown variables at the boundary $x = 0$ and integrate the DAEs governing the first region from $x = 0$ to $x = l_p$. The known boundary conditions at $x = 0$ are solid-phase potential and its flux. The unknown conditions (liquid-phase potential and solid-phase concentration) at first boundary, $x = 0$ are

Table 3
Parameters used for the simulation

Parameters	Values
Electrolyte concentration, c	1000 mol/m ³
Electrolyte conductivity, κ	0.212855 S/m
Solid-phase conductivity, σ	100 S/m
Radius of the particle, R_p	2×10^{-6} m
Specific electrode area, a_p and a_n	885000 and 723600 m ² /m ³
Li ion concentration in particle, $c_{s,\text{max,p}}$ and $c_{s,\text{max,n}}$	25545.01 and 26127.58 mol/m ³
Solid-phase diffusion, $D_{s,p}$ and $D_{s,n}$	1×10^{-14} and 3.9×10^{-14} m/s ²
Reaction rate constant, k_p and k_n	2.334×10^{-11} and 5.0307×10^{-11} mol/(mol/m ³) ^{1.5}
Thickness of Electrodes, l_p and l_n	80×10^{-6} and 88×10^{-6} m
Thickness of separator, l_s	25×10^{-6} m
Discharge current density, I	7.5–150 A/m ²
Transference number, t_+	0.363
Porosity of electrodes, ϵ_p and ϵ_n	0.365 and 0.485
Porosity of separator, ϵ_s	0.724
Volume fraction of fillers, $\epsilon_{f,p}$ and $\epsilon_{f,n}$	0.025 and 0.0326

assumed and then shooting method is performed to the first interface, $x = l_p$ to find the values at second interface, $x = l_p + l_s$. Since the solid-phase potential flux at the first interface is known, it can be used as the shooting criterion. Before integrating the governing equations for first region, one needs to solve for the unknown solid-phase surface concentration corresponding to the other known and guessed values using a nonlinear algebraic solver. This will ensure the consistency of the converged initial values. The numerical values converged at the first interface is significant as it maintains the continuity among the regions.

2. Use the converged values at the interface $x = l_p$ as initial values and integrate the governing equation in the separator from $x = l_p$ to $x = l_p + l_s$. This value at the second interface $x = l_p + l_s$ will serve as fixed and known initial condition for further integration up to $x = L$ ($L = l_p + l_s + l_n$). Usually the governing equation in the separator can be solved easily and a closed-form solution is used.
3. The shooting method similar to the one followed in first region is adopted in the third region to meet the physical constraint imposed by solid-phase potential at the second boundary, $x = L$, i.e. solid-phase potential flux should match $-i_{app}/\sigma_{eff,n}$. The integration for third region stops when this flux at the second boundary meets the required tolerance (10^{-4}).

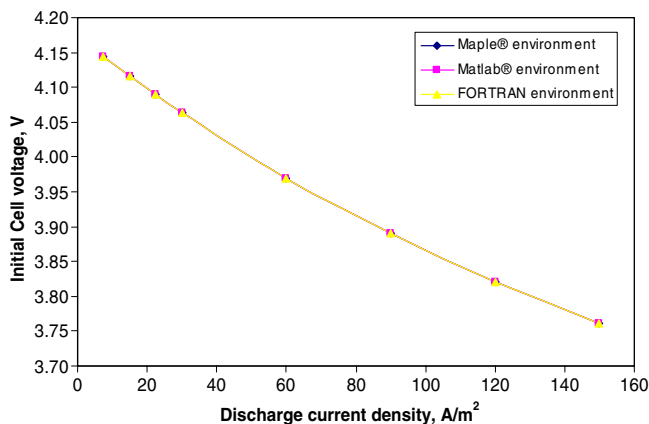


Fig. 3. Comparison of different solvers used for predicting potential loss due to overpotential as a function of discharge current density using the proposed initialization method.

The above scheme is simple and easy to program on a computer using any simulation environment with less computational cost (Fig. 2). By following this procedure, a closed-form solution is also possible for the model equation governing the separator. This further assists in increasing the computation efficiency of the proposed scheme. The steady-state lithium-ion battery model in Table 2 is solved for initial values using the proposed initialization method in three different simulation environments.

The numerical results obtained for the initial cell voltage as a function of discharge current density is shown in Fig. 3 for various environments. The initial condition obtained for solid-phase potential using different simulation environments match on top of each other as expected. The corresponding computation time required for initialization in different simulation environments (1.7 GHz processor and 1 GB RAM) are also given in Table 4. It can be seen that the FORTRAN and DASSL combination works well and can predict the initial condition within a few milliseconds. The computation in other two environments, namely Matlab’s® built-in solver and Maple’s® built-in solver, require a few seconds for successful initialization. The high performance computing language Matlab® out performs the symbolic language Maple® by more than half of the computation cost. However, the proposed method needs only a very few seconds for initialization even while using

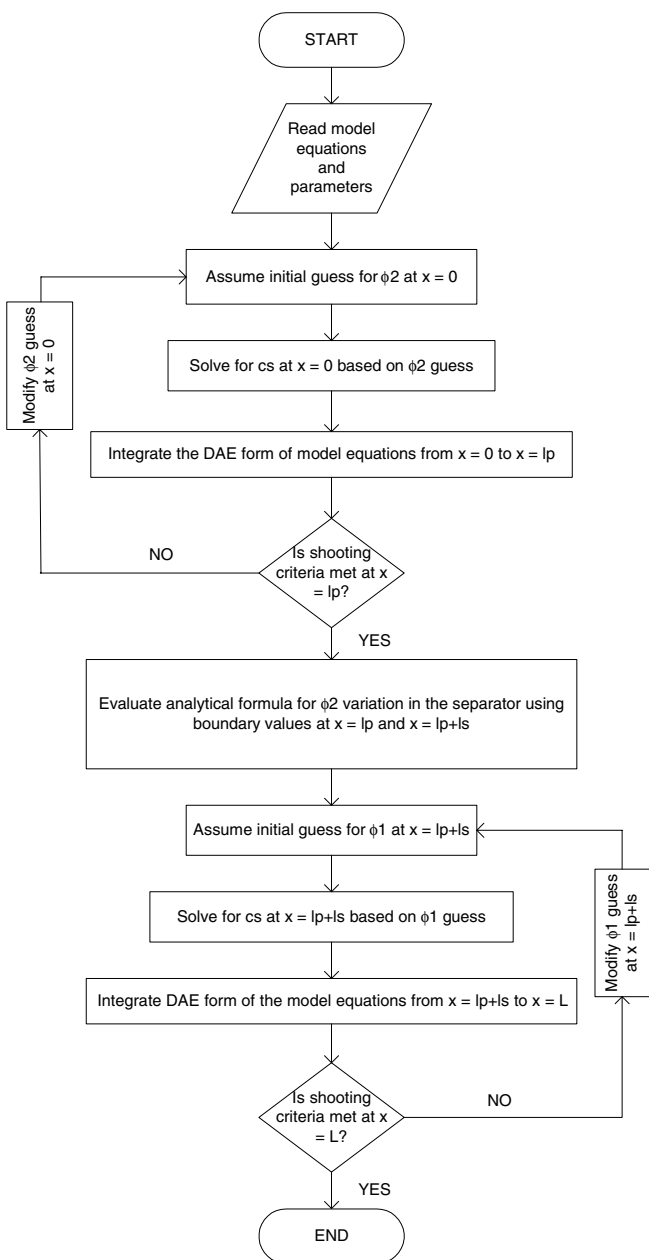


Fig. 2. Flow chart for the proposed computation scheme.

Table 4
Computation time for initialization using the proposed method

Discharge rate	FORTRAN DASSL (ms)	Matlab® in-built solver (s)	Maple® in-built solver (s)
C/4	15.6	1.0	3.5
C/2	15.6	1.0	3.5
3C/4	15.6	1.2	3.6
1C	15.6	1.3	3.6
2C	15.6	1.3	3.7
3C	15.6	1.5	3.8
4C	15.6	1.5	3.9
5C	15.6	1.5	4.0

a computer algebra system. The initial values for dependent variables in polynomial form that best fit the simulation results are expressed below. For the positive electrode:

$$\Phi_1(x) = 4.246 - 2.402 \times 10^4 (I_p - x)^2 + 0.559 \times 10^9 (I_p - x)^3 - 0.624 \times 10^{13} (I_p - x)^4 + 0.266 \times 10^{17} (I_p - x)^5, \quad (1)$$

$$\Phi_2(x) = 0.0005 - 0.132 \times 10^8 x^2 + 0.898 \times 10^{12} x^3 - 0.201 \times 10^{17} x^4 + 0.153 \times 10^{21} x^5, \quad (2)$$

$$c_s(x) = 25548.5 - 0.121 \times 10^7 x + 0.892 \times 10^{11} x^2 - 0.225 \times 10^{16} x^3 + 0.184 \times 10^{20} x^4. \quad (3)$$

For the separator:

$$\Phi_2(x) = 0.055 + \frac{i_{app}}{\kappa_{eff,s}} (I_p - x). \quad (4)$$

For the negative electrode:

$$\Phi_1(x) = 0.182 + 1.88 \times 10^4 (I_p + I_s - x)^2 - 0.319 \times 10^9 (I_p + I_s - x)^3 - 0.279 \times 10^{13} (I_p + I_s - x)^4 + 0.988 \times 10^{16} (I_p + I_s - x)^5, \quad (5)$$

$$\Phi_2(x) = 0.108 - 0.447 \times 10^7 (L - x)^2 + 0.152 \times 10^{12} (L - x)^3 - 0.179 \times 10^{16} (L - x)^4, \quad (6)$$

$$c_s(x) = 25305.363 + 0.2 \times 10^8 x - 0.184 \times 10^{12} x^2 + 0.75 \times 10^{15} x^3 - 0.115 \times 10^{19} x^4. \quad (7)$$

The above equations, Eqs. (1)–(7) can be directly plugged into the computer code that uses popular DAE solvers like DASSL, GAMD, RADAU, *etc.* However, if the solver needs initial values for time derivatives of the algebraic or differential variables, they have to be solved separately. It can be noted that the initial profile governing the separator is a closed-form solution. Since the initial values obtained are exact, it can ensure successful and rapid simulation. The important feature of the proposed procedure is that it requires only 15 ms for initialization in a FORTRAN environment that includes solving and printing the results. This unique characteristic of the proposed approach puts forward the developed methodology to today's demanding simulation requirements such as parameter estimation, on-board battery monitoring, on-line optimization of charge/discharge cycles, *etc.*

3. Conclusion

In this paper, a simple and rapid method for consistent initialization of secondary battery models is proposed. This

technique is based on a shooting method and has been described and demonstrated using an advanced battery model that is represented by coupled nonlinear multiple PDEs. It is found that the method requires only a few milliseconds to initialize a rigorous lithium-ion battery model and could provide exact and consistent initial values. Using the proposed method, the potential loss due to overpotential is plotted as a function of discharge rate in various simulation environments. The computation time is also compared to validate the accurate and rapid initialization properties of the proposed method. The proposed method is suitable for emerging applications such as on-line optimization, on-board monitoring or real time simulation because of its rapidity and consistency with no programming difficulties. Also, the future publications will describe combination of discretization in time (t) and shooting in the x -direction for rapid simulation of discharge curves for batteries.

Acknowledgement

The authors are thankful for the partial financial support of this work by the US Army communications Electronics Command (CECOM) through the project on Advanced Portable Power Institute.

References

- [1] K.E. Brenan, S.L. Campbell, L.R. Petzold, *Numerical Solution of Initial Value Problems in Differential Algebraic Equations*, second ed., SIAM, 1996.
- [2] F. Iavernaro, F. Mazzia, *Appl. Num. Math.* 28 (1998) 107.
- [3] E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-algebraic Problems*, second ed., Springer-Verlag, 1996.
- [4] M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, J.-M. Tarascon, *J. Electrochem. Soc.* 143 (1996) 1890.
- [5] Y. Zhang, H.Y. Cheh, *J. Electrochem. Soc.* 146 (1999) 850.
- [6] B. Wu, R.E. White, *Comput. Chem. Eng.* 25 (2001) 301.
- [7] S. Santhanagopalan, Q. Guo, P. Ramadass, R.E. White, *J. Power Sources* 156 (2006) 620.
- [8] E.C. Biscaia Jr., R.C. Vieira, *Comput. Chem. Eng.* 25 (2001) 1299.
- [9] R. Lamour, *Comput. Math. Appl.* 50 (2005) 1125.
- [10] V.R. Subramanian, V.D. Diwakar, D. Tapriyal, *J. Electrochem. Soc.* 152 (2005) A2002.
- [11] P. Ramadass, P.M. Gomadam, R.E. White, B.N. Popov, *J. Electrochem. Soc.* 151 (2004) A196.