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A Model for Battery Lifetime Calculation Implementable in Circuit Simulators

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Abstract

For pure electrical propelled vehicles, PEVs, a proper battery model is critical in order to estimate State of Charge, SOC, therefore enabling predicting performance and ensuring safe battery operation. Present methods can be classified as electrochemical, electrical equivalent circuits, stochastic and analytical, these last ones based on solution of Partial Differential Equations. These methods are somehow computationally intensive, prejudicing their application in Battery Management Systems. Some ones do not accurately predict battery SOC and most of them are not applicable in electrical circuit simulators. This paper presents a model, based on Fick's laws, capable of an accurate prevision of battery lifetime, i.e. time until battery is empty, and implementable in any circuit simulator. Proposed model behaviour is analysed using PSIM and MATLAB and validated with experimental results.

Keywords: Battery modelling and simulation, FEM, Diffusion, Parameters optimization, SOC calculation.

1 Introduction

With the near future proliferation of Electrical and Hybrid Electrical Vehicles, EVs/HEVs, battery modelling and simulation is a crucial task in order to drive range estimation, as well as safe operation. Therefore accurate models capable of running in real time are a need. The model must allow at capturing the two principal nonlinear effects: rate capacity and recovery. Rate capacity means that real battery capacity lowers during high discharges. Recovery effect is associated with the fact that with light or no discharge the battery seems to increase its capacity.

Pursuing these tasks several battery models have been developed that are usually classified in the following four types: electrochemical, electrical equivalent circuit models, stochastic and analytical. References [1] to [9] present formulations associated to these models.

In this paper it is proposed a physical based model which accurately predicts battery lifetime. Model is implemented and simulated using PSIM and MATLAB. Simulations and experimental results for several load currents are presented for validation purposes.

The paper is organized in the following way: Section 2 presents model derivation. Section 3 deals with parameter evaluation. Simulation and experimental results are compared in Section 4 for model validation. Finally, in Section 5, they are presented paper conclusions.

2 Model Derivation

This section introduces simplified battery physics in order to obtain a model able to predict time until battery is empty taking into account rate capacity and recovery effects. The formulation presented in [1], [2] and [3] is adopted.

All batteries have two electrodes, namely anode and cathode, structured with an electrolyte material. Anode releases electrons and cathode gets electrons during battery load. In operation

electrode reactions involving electrons, *e*, oxidized and reduced species, *O* and *R*, are assumed to be represented by:

Cathode $O+e=R$ (1)

Anode $R=O+e$ (2)

At equilibrium it is assumed that all species are equally distributed in the electrolyte. For a battery load current, flowing in/out battery terminals, this will induce a gradient concentration near electrodes. Loading battery results in a diminution of concentration near electrodes. Stopping electron flux will enable concentration recover due to diffusion. As soon as electrode concentration is bellow a certain level battery operation can no longer be sustained. So, this formulation enables to emulate current gradient and battery recovery effects. Therefore it is adopted the model in 1-D diffusion of active materials in battery electrolyte as presented by Rakhmatov et al. [1].
The model assumes a symmetrical battery with equal behaviour for oxidized and reduced species, *O* and *R*. Consequently it can be worked out only one electrode and half of the electrolyte length, *L*.
1-D electrolyte species concentration at any time, t, (t>0) and distance, x, (0<x<L) are given by Fick's Laws:

$$-J(x,t)=D\frac{\partial C(x,t)}{\partial x} \quad (3)$$

$$\frac{\partial C(x,t)}{\partial t}=D\frac{\partial^2 C(x,t)}{\partial x^2} \quad (4)$$

$J(x,t)$ is species flux in electrolyte, D a diffusion coefficient and $C(x,t)$ species concentration.
Boundary condition at $x=0$ is taken from Faraday's law that relates current and flux at electrode surface:

$$\frac{i(t)}{\nu FA}=D\frac{\partial C(x,t)}{\partial x}\Big|_{x=0} \quad (5)$$

A is electrode area and F Faraday's coefficient; ν is the number of electrons associated to the reaction in the electrode.
Flux at the other boundary, $x=L$, is zero:

$$0=D\frac{\partial C(x,t)}{\partial x}\Big|_{x=L} \quad (6)$$

If current i(t) is constant, a general solution for PDE equations (3) and (4) is possible, subjected to the boundary conditions (5) and (6) and using Laplace transform [1] and [2].
Paper approach tries a solution using a finite difference formulation with n uniformly spaced elements of width $\frac{L}{n}$. Firstly it is normalized the spatial variable x into $x'=\frac{x}{L}$ and used charge, Q, instead of ion concentration, $Q=CA\nu F$.
Equations (3), (4), (5) and (6) become:

$$-J(x',t)A\nu F=\frac{D}{L}\frac{\partial Q(x',t)}{\partial x'} \quad (7)$$

$$\frac{\partial Q(x',t)}{\partial t}=\frac{D}{L^2}\frac{\partial^2 Q(x',t)}{\partial x'^2} \quad (8)$$

$$i(t)=\frac{D}{L}\frac{\partial Q(x',t)}{\partial x'}\Big|_{x'=0} \quad (9)$$

$$0=\frac{D}{L}\frac{\partial Q(x',t)}{\partial x'}\Big|_{x=1} \quad (10)$$

Charge, $Q(x',t)$, at $x'=0$ ($x=0$) and $x'=1$ ($x=L$) are denoted by $Q_1(t)$ and $Q_n(t)$. At any other element at $x'=(k-1)\alpha$ $(1<k<n)$ charge is $Q_k(t)$.

Discretizing the domain with a step size $\alpha=\frac{1}{n}$ and using a centered finite difference approximation to the second order spatial derivative:

$$\frac{\partial^2 Q(x',t)}{\partial x'^2}=\frac{Q(x'+\alpha,t)-2Q(x',t)+Q(x'-\alpha,t)}{\alpha^2}$$

The set of equations (11) is established.
These equations in matrix form are presented in (12).

$$
\begin{aligned}
&\frac{\partial Q_1(t)}{\partial t} = \frac{1}{\alpha}\left[\frac{D}{\alpha L^2}\left(Q_2(t) - Q_1(t)\right) - i(t)\right] \\
&\frac{\partial Q_2(t)}{\partial t} = \frac{1}{\alpha}\left[\frac{D}{\alpha L^2}\left(\left(Q_3(t) - Q_2(t)\right) - \left(Q_2(t) - Q_1(t)\right)\right)\right] \\
&\cdots \\
&\cdots \\
&\frac{\partial Q_{n-1}(t)}{\partial t} = \frac{1}{\alpha}\left[\frac{D}{\alpha L^2}\left(\left(Q_n(t) - Q_{n-1}(t)\right) - \left(Q_{n-1}(t) - Q_{n-2}(t)\right)\right)\right] \\
&\frac{\partial Q_n(t)}{\partial t} = \frac{1}{\alpha}\left[\frac{D}{\alpha L^2}\left(-\left(Q_n(t) - Q_{n-1}(t)\right)\right)\right]
\end{aligned}
\tag{11}
$$

$$
\begin{bmatrix}
\frac{\partial Q_1(t)}{\partial t} \\
\frac{\partial Q_2(t)}{\partial t} \\
\frac{\partial Q_3(t)}{\partial t} \\
\cdots \\
\frac{\partial Q_{n-1}(t)}{\partial t} \\
\frac{\partial Q_n(t)}{\partial t}
\end{bmatrix}
= \frac{1}{\alpha}\frac{D}{\alpha L^2}
\begin{bmatrix}
-1 & 1 & \cdots & \cdots & \cdots & 0 \\
1 & -2 & 1 & \cdots & \cdots & 0 \\
0 & 1 & -2 & 1 & \cdots & 0 \\
\cdots & \cdots & & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & \cdots & \cdots & 1 & -2 & 1 \\
0 & & & 0 & 1 & -1
\end{bmatrix}
\begin{bmatrix}
Q_1(t) \\ Q_2(t) \\ Q_3(t) \\ \cdots \\ \cdots \\ Q_{n-1}(t) \\ Q_n(t)
\end{bmatrix}
- \frac{1}{\alpha}
\begin{bmatrix}
i(t) \\ 0 \\ 0 \\ \cdots \\ \cdots \\ 0 \\ 0
\end{bmatrix}
\tag{12}
$$

$$
\begin{aligned}
&C_1\frac{\partial V_1(t)}{\partial t} + \frac{\left(V_1(t) - V_2(t)\right)}{R_{12}} + i(t) = 0 \\
&C_2\frac{\partial V_2(t)}{\partial t} + \frac{\left(V_2(t) - V_1(t)\right)}{R_{12}} + \frac{\left(V_2(t) - V_3(t)\right)}{R_{23}} \\
&C_3\frac{\partial V_3(t)}{\partial t} + \frac{\left(V_3(t) - V_2(t)\right)}{R_{23}} + \frac{\left(V_3(t) - V_4(t)\right)}{R_{34}} \\
&\cdots \\
&\cdots \\
&C_{n-1}\frac{\partial V_{n-1}(t)}{\partial t} + \frac{\left(V_{n-1}(t) - V_{n-2}(t)\right)}{R_{n-1n-2}} + \frac{\left(V_{n-1}(t) - V_n(t)\right)}{R_{n-1n}} = 0
\end{aligned}
\tag{13}
$$

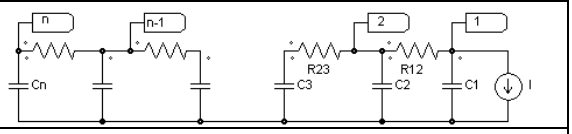

Figure 1: Electrical circuit for PDE solution.

Considering the circuit presented in Figure 1, equations (13) are established (naming voltage at nodes $V_1(t)$, $V_2(t) \ldots V_n(t)$).

These equations are similar to (11). Therefore this electrical circuit models charge in space $0 < x' < 1$ as voltage in circuit nodes. The number of nodes equals the number of elements, n , with values for R_{ij} and C_k being a function of α , L and D .

So it is got an approximate solution of PDE equations (7) and (8), subjected to the boundary conditions (9) and (10), using an electrical circuit made of a set of *RC* nets, like the one in Figure 1, with battery load attached to the first node ($x' = x = 0$). Next section presents the approach used for evaluation of values associated to R_{ij} and C_k .

3 Model Parameters

The model obtained in Section 2 for solution of Fick's Laws uses an electrical circuit made of a set of n RC nets whose values are dependent on physical parameters which are usually unknown. So, these values must be estimated.

The estimation method is supported on an optimization algorithm based on Simulated Annealing, SA, [10], [11], [12], working firstly a solution using only two nodes. It is needed to obtain values for two capacitors and a resistor as result.

SA minimizes a function typically established as the energy of the system in study.

It starts with an initial solution for the problem, usually a vector. With this solution the energy is calculated for this first state.

SA then generates a new solution in the neighbourhood of the initial one, computing the new energy state.

Subsequently SA uses a probabilistic function in order to decide whether it moves to the new solution, or not. This usually prevents that the algorithm is trapped at some local minimum because it can be accepted a worst solution, depending on the probability. This probabilistic function uses the energy of the two states being analysed as well as a time varying parameter, generally adopted as temperature, T, which is updated between iterations. Thus, as the algorithm evolves the probability of acceptance of worst solutions is decreased.

To adopt SA demands for:

- An initial solution;
- A function associated to system energy;
- A neighbourhood generator;
- A probabilistic function to move between solutions.

For the initial solution they are produced several sets of random values, S_i, for R_{ij} and C_k. In this particular case sets of resistors, R_{12}, and capacitors C_1 and C_2 are created. From these ones it is chosen the set that minimizes system energy.

Applied function for calculus of system energy is the mean of the relative error between model simulation and experimental results. These are obtained for constant currents. Section 4 presents the setup used for experiments.

Some concepts from Genetic Algorithms are used for designing neighbourhood generator. New solution candidates, S_{i+1}, are generated randomly from old ones, S_i, inside a limited grid given by $(1-0.5)S_i < S_{i+1} < (1+0.5)S_i$. New candidates are generated varying only one of the elements of the vector in each try, starting by C_1. Having the best C_1 in this neighbourhood algorithm proceeds for next element of the solution vector, R_{12}, and so on.

The function used to calculate the probability, associated to acceptance of the new solution, has value one if the obtained error is less than the best error until now. If not, the new solution can still be accepted if:

$$\exp\left[-\frac{actualerror - besterror}{T}\right] \qquad (14)$$

is less that a randomly generated number. T is known as temperature and is updated at each iteration using:

$$T_{i+1} = \beta T_i \qquad (15)$$

β has typically a value approaching 0.9.

The SA algorithm was developed and implemented as a MATLAB script.

4 Model Validation

4.1 Experimental Setup

Figure 2: Experimental setup.

The model validation is based on constant discharge currents. The built setup is shown in Figure 2. It uses a B&K Precision model 8510 electronic load, for programmed discharge and voltage acquisition, and a NI DAQ PCI 6024E card for temperature and current acquisition. Tests used a General Electronics Battery Co., Ltd. Lithium Battery, Model 10059156SH5. (3.7V, 11000mAh). The experiments are done inside a

climatic chamber model Fitoclima 3600 EDTU from Aralab in order to work with a well-defined temperature. The experimental procedure consists in full charging the battery followed by a rest period. Then the battery is discharged to its cut-off voltage, using several dc current profiles, and the time spent from full charge to cut-off is measured.

4.2 Model Simulation

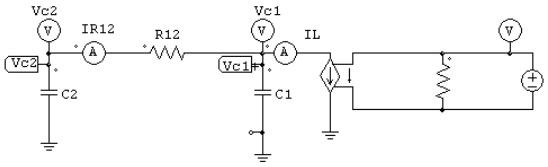

Figure 3: Simulation circuit.

Figure 3 presents PSIM circuit used for simulation analysis. Model parameters are estimated following the procedure presented in Section 4. The battery is assumed fully discharged when voltage at node 1, $V_1(t)$, is zero. Remember that this voltage measures concentration at the electrode ($x' = x = 0$). Time for full discharge, for the different current profiles, is then extracted from the results file.

4.3 Results

Table 1: Experimental and simulated results for dc currents

Current (mA)	Experimental Lifetime (s)	Simulated Lifetime (s)	Error (%)
1085	35256	36274	2,89
1086	38217	36274	5,08
2170	18312	18025	1,57
2185	17615	17899	1,61
2186	17886	17891	0,03
2730	14514	14282	1,60
3285	11761	11832	0,60
5484	6534	6997	7,09
5485	6937	6996	0,85
5490	6813	6989	2,58
6586	5783	5788	0,09
8788	4025	4283	6,41
9885	3869	3783	2,22
10989	3510	3380	3,70
10991	3432	3379	1,54
14990	2274	2418	6,33

Experimental and simulated times for battery full discharge for several constant current loads are shown in Table 1.

Figure 4 shows the error between simulation and experimental discharge times. As it can be observed the relative error is small: For constant current discharge the maximum error is 7.09%, the minimum 0.03% and the mean relative error 2.76%.

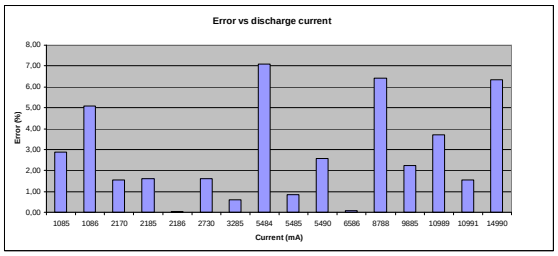

Figure 4: Experimental versus simulation results.

5 Conclusions

This paper presents a battery model based on a Finite Difference solution of Fick's law that is applicable in any circuit simulator.

The model uses a set of *RC* nets whose values are estimated with a heuristic that uses experimental results and is based on a Simulated Annealing Algorithm. The number of *RC* nets is a compromise between accuracy and computational time.

The model has been tested with one *RC* net and obtained results show that it can predict discharge time with mean errors around 3%.

In future work authors intend to expand this model in order to become it able to predict battery terminal voltage. Authors also aim at improving the model using an approach with variable *RC* net elements, which are current controlled, in order to maximize accuracy.

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