



## Short communication

# Comparison of lumped diffusion models for voltage prediction of a lithium-ion battery cell during dynamic loads



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## HIGHLIGHTS

- Battery modelling for Battery Management Systems.
- Dynamic prediction of battery voltage without any knowledge of the internal chemistry.
- Comparison of various lumped models.
- Including a concentration overpotential improves model accuracy.
- Resistor-Capacitor (RC) pairs may be replaced by particle diffusion equations.

## A B S T R A C T

Three different time-dependent lumped battery models are presented, using a limited set of only either three or four fitting parameters. The models all include one linear (resistive), one non-linear (kinetic) and one time-dependent element, the latter describing the diffusive processes in the battery. The voltage predictive capabilities of the models versus experimental dynamic load data for a plug-in hybrid vehicle battery are compared. It is shown that models based on a diffusion equation in an idealized particle perform similarly to a model based on an RC (resistive-capacitor) pair. In addition, by exchanging the RC element by a diffusion equation in an idealized particle it is also shown that it is possible to reduce the number of needed fitting parameters by one.

## 1. Introduction

Lithium-ion batteries (LIBs) are widely employed as storage for electric energy in electric and hybrid electric vehicles. On board the vehicle, the battery management system (BMS) is responsible for assessing various battery state variables such as energy content, capability to deliver power and general “health” condition, commonly referred to as state-of-charge (SOC), state-of-power (SOP) and state-of-health (SOH), respectively [1]. Whereas SOC and SOH have been extensively studied in scientific literature, methods for SOP prediction and assessment seem to have been less explored [2].

State-determination techniques commonly make use of mathematical models, to higher or lower degrees of complexity, for describing the battery. Physics-based LIB models, the most well-known is most likely the one developed by Newman and co-workers in the 1990's [3], make use of partial differential equations for describing and coupling the transport of electrons, ions and other reacting species in the various phases (electrolyte, electrodes and metal current conductors). Such models are typically one-dimensional across the layers of the battery

cell, with an additional dimension used to describe the diffusion of solid lithium within the electrode particles, comprising a “psuedo-2D” (P2D) approach. Physics-based models have been successful in capturing the dynamic behaviour of LIBs for various operational cases, and the detailed description about the electrode environment makes it easy to, for instance, add parasitic reactions for ageing and capacity fade modelling. A drawback is however the need for detailed knowledge about the characteristics of the individual electrode, separator and electrolyte materials, which can usually only be obtained by extensive experimental work, although there is work in progress to determine some of these parameters by ab-initio-based multiscale approaches [4,5]. Around 40 parameters are typically needed for setting up a model, and this often makes the model unpractical for engineering applications where knowledge about the internal battery chemistry may be limited. For low and moderate currents, the Newman model can be simplified by using a single-particle approach [6,7] wherein the current distribution effects within the porous electrodes and concentration changes in the electrolyte are neglected. This approach reduces the total number of needed parameters somewhat, but setting up even a

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simplified physics-based model and fitting it to battery cell data can still be a daunting task. The computational load of a physics-based model may also be comparably high since the need to resolve concentration and potential gradients in the electrodes and electrode particles may require a fine computational mesh in the finite element or finite difference numerical schemes used when solving the model.

A different class of models stems from the equivalent circuit (EC) approach, wherein a number of simple circuit components such as resistors, capacitors and inductors are coupled together into a circuit with dynamic voltage characteristics that resemble those of an operating battery. An EC model typically make use of far less parameters than a physics-based model, and has a generally lower computational load. A disadvantage with an EC model is however that there is no way, apart from the case when only a few circuit components are included, to directly associate an EC component to a certain part of, or phenomena in, the battery. An additional complication is that seemingly differently designed circuits may result in identical mathematical behaviour [8].

Apart from the two modelling approaches mentioned above, there are also other techniques available for battery modelling such as self-learning neural networks. Combining elements from both approaches into hybrid methods is also possible [9] (the single-particle model could actually be seen as an EC with diffusion resistance elements [7]).

Regardless of modelling technique used, the BMS will have to perform continuous parameter estimation of the parameters used in the battery state-assessment model(s) used on-board [1]. To facilitate parameter estimation, a requisite for a model is hence not only its accuracy, and low computational load, but also that the number of parameters is small, and that the parameters are reasonably uncorrelated, i.e. that they operate mainly on different time scales and/or affect the voltage differently depending on the magnitude of the battery load current.

This paper investigates three different variants of a lumped battery model, all of them encompassing a linear ohmic resistance, a non-linear charge transfer resistance and a diffusion impedance. Two different approaches for modelling the diffusion impedance are investigated: 1) using a common Resistor-Capacitor (RC) circuit element or 2) using a diffusion equation in an idealized particle. The models are fitted to experimental battery data, and the difference in results when validating the models to a second set of data are compared and discussed, with the evaluation of the models having a SOP application in mind, thus focusing on the ability to predict the voltage for a given load cycle. (For experimental reasons and in order to validate the models, the formulations are however based on a given current load input, rather than power.)

## 2. Mathematical model

The three different models investigated can be described as lumped semi-empirical models, defining physics-based voltage losses (overpotentials) pertinent to ohmic, activation and concentration (diffusion) losses. A list of the symbols used in the model are shown in Table 1.

The model defines the time-dependent evolution battery cell voltage,  $E_{\text{batt}}$  (V) when subject to a time-dependent battery current load  $I_{\text{batt}} = I_{\text{batt}}(t)$  (A) using the equation

$$E_{\text{batt}} = E_{\text{OCV}}(\text{SOC}) + \eta_{\text{ohm}} + \eta_{\text{act}} + \eta_{\text{conc}} \quad (1)$$

where  $E_{\text{OCV}}(\text{SOC})$  (V) is the battery open circuit voltage (OCV) as function of SOC (1), the battery state-of-charge.

The SOC depends on the battery current as

$$\frac{d\text{SOC}}{dt} = \frac{I_{\text{batt}}}{Q_{\text{batt}}} \quad (2)$$

where  $Q_{\text{batt}}$  (C) is the battery capacity.

The overpotential due to ohmic losses in the battery,  $\eta_{\text{ohm}}$  (V), is defined as

**Table 1**  
Symbols used in the model.

Symbol	Unit	Description
$C$	F	Capacitance
$d$	1	Dimension number
$E_{\text{batt}}$	V	Battery voltage
$E_{\text{OCV}}$	V	Battery open circuit voltage
$F$	$\text{Cmol}^{-1}$	Faraday's constant, 96485 C/mol
$I_{\text{batt}}$	A	Battery current
$I_0$	V	Exchange current
$K$	V	Battery voltage dependency on surface SOC
$Q$	C	Battery capacity
$R$	$\text{J}(\text{molK})^{-1}$	Molar gas constant, 8.1345 J/(mol K)
$R_c$	Ohm	Resistance in RC circuit element
$R_{\text{ohm}}$	Ohm	Ohmic resistance
$S$	1	Local SOC in particle
SOC	1	Battery SOC
$T$	K	Temperature
$X$	1	Particle spatial variable
$\sigma$	V	Standard deviation
$\eta_{\text{act}}$	V	Activation overpotential
$\eta_{\text{conc}}$	V	Concentration overpotential
$\eta_{\text{ohm}}$	V	Ohmic overpotential
$\tau$	s	Diffusion time constant

$$\eta_{\text{ohm}} = R_{\text{ohm}} I_{\text{batt}} \quad (3)$$

where  $R_{\text{ohm}}$  (ohm) is the ohmic resistance.

Introducing a non-linear term in the current-voltage dependency has been shown to improve the accuracy of SOP assessment models [1]. In this work we include an activation overpotential due to charge transfer processes in the battery,  $\eta_{\text{act}}$  (V), defined using an inverted Butler-Volmer equation (using anodic and cathodic symmetry factors equal to 0.5) as

$$\eta_{\text{act}} = \frac{2RT}{F} \operatorname{arcsinh} \left( \frac{I_{\text{batt}}}{2I_0} \right) \quad (4)$$

where  $R$  (8.31 J/(molK)<sup>-1</sup>) is the molar gas constant,  $F$  (Cmol<sup>-1</sup>) is Faraday's constant,  $T$  (K) the temperature and  $I_0$  (A) the exchange current. Equation (4) represents the non-linear relation between current and potential, commonly found in electrochemical systems.

The third source of voltage losses are due to finite transport rates of reacting material in the battery, and power prediction has been shown to be improved also by adding a contribution stemming from a diffusion impedance [10]. We name this voltage loss the concentration overpotential  $\eta_{\text{conc}}$  (V). Three different models for determining  $\eta_{\text{conc}}$  (V) are used in this paper: the RC model, the  $K\tau$  model and the  $\tau$  model. All the concentration overpotential models make use of a time constant parameter  $\tau$  (s).

The RC model is defined using a Resistor-Capacitor (RC) pair, coupled in parallel. This circuit element is commonly used in EC models. The resulting overpotential is defined by the following ordinary differential equation (ODE)

$$\tau \frac{d\eta_{\text{conc}}}{dt} + \eta_{\text{conc}} = R_c I_{\text{batt}} \quad (5)$$

where  $R_c$  (ohm) is the resistance. The time constant for this model is related to  $R_c$  and  $C$  (F), the capacitance of the RC circuit, according to

$$\tau = R_c C \quad (6)$$

The RC model hence uses  $R_{\text{ohm}}$ ,  $I_0$ ,  $\tau$  and  $R_c$  as fitting parameters.

The  $K\tau$  model for the concentration overpotential resembles in many ways the single-particle-model [7], with the additional assumption that only one of the electrodes contributes to the diffusion-related voltage losses on the cell level. For this case the two electrode particles in the single particle model can be replaced by one particle only. The diffusion equation solving for a local particle state-of-charge variable  $S$  (1) is defined on a one-dimensional geometry, using a dimensionless

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