

Options for Coupled Thermal-Electric Modeling of Battery Cells and Packs

Scott Peck
ThermoAnalytics Inc.

Aditya Velivelli
Exa Corp.

Wilko Jansen
Jaguar & Land Rover

ABSTRACT

Integration of advanced battery systems into the next generation of hybrid and electric vehicles will require significant design, analysis, and test efforts. One major design issue is the thermal management of the battery pack. Analysis tools are being developed that can assist in the development of battery pack thermal design and system integration. However, the breadth of thermal design issues that must be addressed requires that there are a variety of analysis tools to address them efficiently and effectively.

A set of battery modeling tools has been implemented in the thermal modeling software code PowerTHERM. These tools are coupled thermal-electric models of battery behavior during current charge and discharge. In this paper we describe the three models in terms of the physics they capture, and their input data requirements. We discuss where the capabilities and limitations of each model best align with the different issues needed to be addressed by analysis. Model outputs are compared with measured data for various analysis scenarios, including simulation of constant current charge/discharge, and response to charge/discharge profiles derived from a standard drive cycle, for both single cell and multi-cell pack configurations. We conclude with recommendations for matching model competencies with analysis requirements.

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INTRODUCTION

A characteristic of Li-ion batteries is complex behavior during charge or discharge. Several fault mechanisms exist if a battery is overheated or operated at too high or too low a voltage. It is important to operate Li-ion batteries within a well-defined performance envelope to avoid degradation in power, capacity, life, and safety. Proper system integration is a key factor in the success of these devices for any application.

Access to verified, validated battery performance models implemented in commercially available CAE software is of great value to end users and battery suppliers, as well as researchers trying to develop better cell designs. The questions facing researchers, suppliers, and users occur on different scales and levels of behavior. These questions can be grouped into three levels: electrode level, cell level, and pack level.

Electrode level models are concerned with the coupled electrochemical diffusion processes involved in ion transport between anode and cathode. Cell level models begin to account for effects occurring in the two dimensions containing the plane (or cylindrical sheet) of the electrodes, such as local potential differences between electrodes, local current density, local capacity, and temperature. Finally, pack level models are concerned not only with local differences over a cell cross-section, but with effects of variations from cell to cell, and with effects related to non-uniform boundary conditions at the interfaces of a pack and the electrical/thermal/structural system it is embedded in.

The electrode, cell, and pack level issues represent a spectrum of design problems needing to be solved for successful adoption of Li-ion battery technology into electric vehicles and other devices. Automotive system integrators will be primarily interested in pack level modeling with a secondary interest in cell models.

Three different battery analysis modules that are designed to address cell and pack level modeling have been incorporated into a commercial thermal solver. Two are based on the NTG (Newman, Tiedemann, and Gu[1,2,3]) parametric model of battery behavior, while the third is based on a parametric model developed at the National Renewable Energy Laboratory (NREL)[4]. The NREL and one of the NTG models are equivalent circuit models, where the electrical behavior of the battery is described in terms of circuit parameters. The second NTG model is a distributed model, in that it describes the current density and voltage distribution over the electrodes of a cell. All three models are based on empirical data, and do not attempt to describe the physics of the electrochemical reaction and charge diffusion from first principles. Each model has relative advantages and disadvantages, and the choice of which to use depends on the goals of the analysis.

DESCRIPTION OF MODELS

In all three models, a shell element mesh is used to represent the thermal domain of the cell. Cell temperatures are computed on this mesh in response to the joule heating produced within the electrode, moderated by material properties and environmental boundary conditions. In the equivalent circuit models, lumped parameter nodes are used for the electrical domain. In the distributed model, additional copies of the geometry are created to represent the electrical domains of the anode and cathode. Voltages are computed on these meshes in response to the imposed current load and internal voltage potential (the open-circuit voltage) distribution.

The electrical computations are done in the thermal solver by taking advantage of the analogy between thermal and electrical phenomena. Thus electrical voltages, currents, and resistances are interpreted by the solver as temperatures, heat flows, and thermal resistances. Special solver modules manage this interpretation, and provide the coupling between the electrical and thermal behavior. This includes heating of thermal components based on currents and resistances, and determination of electrical parameters based on temperatures. Electrical boundary conditions are provided through a combination of user interface (GUI) inputs and data supplied in an auxiliary text file.

NTG Equivalent Circuit Model

The NTG equivalent circuit model describes battery behavior in terms of a voltage source and an internal resistance. The circuit model is shown in Figure 1. There are two parameters: the internal voltage source U , and a series resistance $1/YA$, where A is the area normal to the electrode, and Y is a conductance per unit electrode area. Both U and Y are functions of temperature and depth-of-discharge of the battery. The depth-of-discharge is defined as

$$DoD = DoD_0 - \int_0^t Idt / 3600C \quad (1)$$

where I is the current imposed on the battery (negative for discharge), and C is the capacity of the battery in ampere-hours, integrated from $t = 0$ (time at which the battery has an initial DoD_0) to an arbitrary time (in seconds).

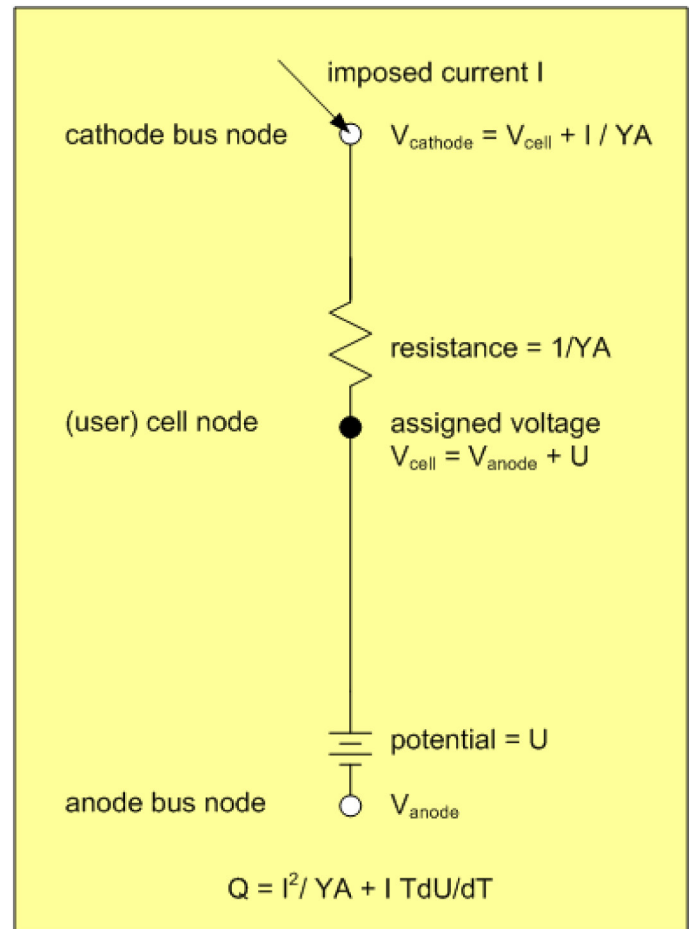


Figure 1. NTG equivalent circuit schematic.

Note the sign convention that current is positive when *into* the cell, so a positive imposed current implies the cell is being charged, while a negative current indicates a discharge.

Bus nodes are used to create connections between cells. Bus nodes are created via the battery text input file. Connections between cells and bus nodes are also created via this file. The battery model enforces conservation of current at all bus nodes, and will adjust bus node voltages to ensure it. Parallel connections of cells are created by identifying a common bus node for the cathode or anode bus nodes of several cells. Series connections are created by specifying a bus node as the anode bus node of one (or more) cells and the same bus node as the cathode bus node of those cells having a series connection. Any combination of series and parallel pack topologies can be specified in this manner. However, it is up to the modeler to provide an electrically valid network.

The heat generated in the battery due to current charge or discharge is the ohmic heating generated due to the internal resistance (I^2/YA), plus the reversible heating produced by the

electrochemical reaction at the electrodes ($ITdU/dT$). In the NTG models, the dU/dT term is restricted to be a constant. In the equivalent circuit model, the total heat is uniformly distributed over the set of geometry representing the thermal model of the individual cell.

NTG Distributed Model

In the NTG distributed model, the circuit equation is effectively applied in parallel on a per unit area basis over the electrode. This is shown in Figure 2. The anode and collector plates, as well as the cell itself, are discretized with two-dimensional meshes, and the local current density is computed as a function of the local voltage difference between anode and cathode, moderated by the conductance per unit area parameter Y , and the local electrochemical potential value represented by U . U and Y are the same parameters as defined for the NTG equivalent circuit model. The voltage distribution on the collector plates is determined by solving Poisson's equation

$$\nabla^2 V = \pm J / \sigma d \quad (2)$$

where V is the voltage on either the anode or cathode, J is the current density (positive from cathode to anode), σ is the electrical conductivity of the collector plate material, and d is the thickness of the collector plate. The positive sign is used for the right-hand side for the anode, and the negative sign for the cathode.

The current density is computed from the NTG model as

$$J = Y[(V_p - V_n) - U] \quad (3)$$

where V_p is the local voltage on the cathode, V_n is the local voltage on the anode, and U and Y are as before.

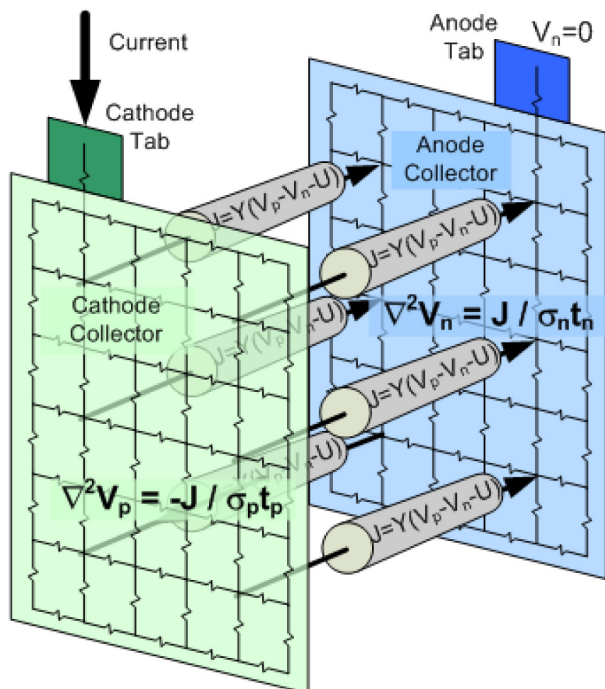


Figure 2. The NTG distributed model.

The NTG distributed model requires that the anode and cathode be represented as geometry in the model, in order that the thermal solver can be used to solve Poisson's equation. Furthermore, the geometry used to represent both the anode and the cathode must be identical to the geometry used for the thermal model of the cell. Electrical connections between cells are modeled either with geometry representing the cell-to-cell connectors, or with 'thermal links', which create a user-specified conductance between designated nodes in the model.

In the NTG distributed model, the depth-of-discharge is computed locally (for each anode/cathode element pair), and so non-uniformities in electrode utilization will be revealed. The local value is computed from

$$DoD = DoD_0 - \int_0^t J dt / 3600 Q_T \quad (4)$$

where J is the local current density in amperes/m², Q_T is the theoretical capacity per unit electrode area of the cell in ampere-hours/m², and t is the time in seconds.

In the distributed model, the heating is computed and applied locally. The heat per unit volume of electrode generated by current transfer between the electrodes is

$$\dot{q}_e''' = \frac{J}{d} \left[V_p - V_n - U + T \frac{dU}{dT} \right] \quad (5)$$

In this context, d is the total thickness of the cell. The model also includes ohmic heating from current flowing in the plane of the collector plates. This heat is computed on a volumetric basis as

$$\dot{q}_c''' = \sigma (\nabla V \cdot \nabla V) \quad (6)$$

in each plate, with σ equal to the electrical conductivity of the collector plate material.

NREL Equivalent Circuit Model

The NREL equivalent circuit model is similar to the NTG equivalent circuit model in that cell behavior is captured in a zero-dimensional lumped parameter model. The equivalent circuit schematic is shown in Figure 3. There are two additional circuit features in this model compared to the NTG model. The first is the addition of 'filter circuits' in series with the voltage source and the internal resistance. The second is the inclusion of an optional resistance used to model a built-in current limiting element found in some cell designs.

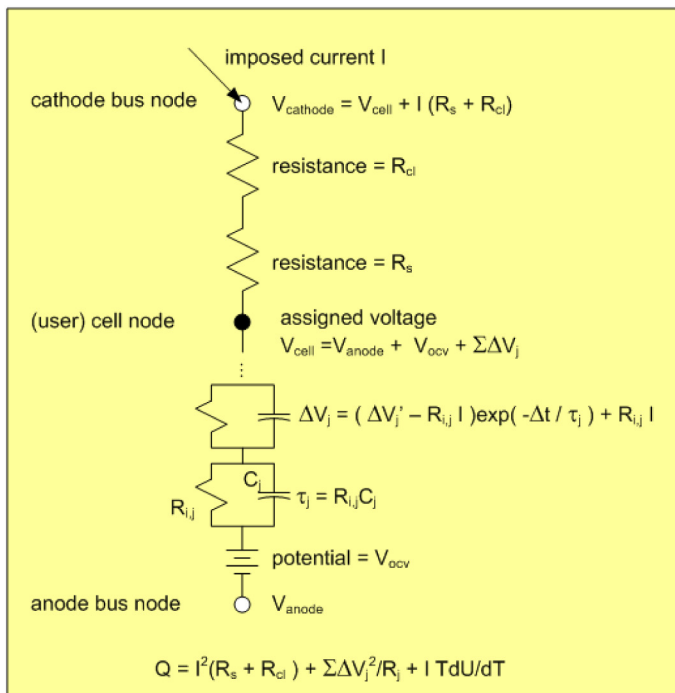


Figure 3. The NREL equivalent circuit schematic.

The filter circuits consist of a series of parallel resistor/capacitor (RC) circuits. These simulate the response a battery exhibits to changes in imposed current that occur, for example, during a drive cycle with transient power demands on the battery pack of a vehicle. The filter circuits are characterized by a resistance R_{ij} and a time constant τ_j . The model accommodates as many filter circuits as needed to capture the transient response of the cell.

The other new circuit feature is the ability to include a current-limiting resistor in the model. Some cells have resistive elements built into them that are highly temperature-dependent. If a fault condition occurs that subjects the cell to a high current, these elements heat up and the resistance increases by several orders of magnitude, thereby limiting the current flow. This resistance is a function of temperature only.

All the other circuit parameters are functions of depth-of-discharge and temperature. In addition to the R_{ij} and τ_j , there is an internal series resistance, denoted in this model as R_s , and a voltage source, denoted V_{ocv} (open cell voltage) here.

The current is again considered positive when it is charging the cell, and the terminal voltage is the sum of all the internal drops from cathode to anode.

Just as the models have different features and capabilities, they have different input requirements. The inputs are of two types: those characterizing cell behavior (i.e., parameterized voltage - current relationships); and those characterizing the cell configuration and connectivity.

NTG Distributed Model Inputs

The inputs for the NTG distributed model fall into the first type, characterizing cell behavior. Of primary importance are inputs describing the U and Y parameters. The inputs describe U and Y in terms of the depth of discharge DoD, and temperature, T. The syntax of the text input file admits defining U and/or Y as a table of data with a single independent variable, either DoD or T, or as a double table of data with two independent variables, or as polynomial curve fits with DoD and/or T as the independent variable. In addition, T can either be the environmental temperature or the cell temperature, depending on how the test data was obtained. U has units of V, while Y is in Siemens/m². These parameters are derived from constant current discharge data (terminal voltage as a function of time) taken at different discharge rates (current densities). The procedure to obtain these parameters is described elsewhere[2], but in essence they are determined by finding the slope (1/Y) and intercept (U) of plots of voltage as a function of current density at different values of DoD.

In addition to the U and Y parameters, the NTG distributed model requires a value for dU_{oc}/dT , in V/K, which is used to compute the reversible heat of the chemical reaction occurring in the electrodes.

The cell capacity is defined with the parameter Q_j , which is the theoretical capacity of the cell per unit area of electrode, in Amp-hr/m².

The joule heating that occurs due to current flow in the collector plates on the anode and cathode are computed using the inputs cathodeConductivity and anodeConductivity, which are the electrical conductivities of the cathode and anode collector plate materials, respectively. These quantities have units of Siemens/m.

Finally, the initial condition for the charge state of the cells in the model is specified via the parameter initialDoD, which must be between zero and one.

Because the NTG distributed model was developed with single cells in mind, there is no provision in the text input file for this model to define connections between multiple cells. However, cells can be connected by creating geometric representations of the bus work in the electrical part of the model, or by creating node-to-node links representing the connections. The current for a cell or pack is specified by imposing a current on the cathode terminal of the cell or pack. (The anode terminal voltage is set to zero in the model.)

NTG Equivalent Circuit Model

The inputs describing cell behavior are the same in the NTG equivalent circuit model as in the distributed model. That is, the same data for U, Y, and dU_{oc}/dT are needed. Since the voltage distribution on the collector plates is not computed in this model, the electrical conductivities of the cathode and anode collectors are *not* needed for this model.