Li-ion battery model with temperature and aging effect

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Abstract

1 The overall modelling goal and assumptions

1.1 Modelling goal

The overall modelling goal is twofold: the basic model should describe the operation of a Li-ion battery at constant temperature without aging effects. The operation of real batteries depends on the temperature and the dynamic usage therefore the extended model should be able to investigate thermal and aging effects too. The model should contain the internal resistance and the capacity of the battery as these two parameters strongly dependent of temperature and aging.

1.2 Modelling assumptions

The following assumptions are made for the basic battery model[1]:

- The internal resistance is supposed to be constant during the charging and discharging and does not vary with the amplitude of the current.
- The parameters are deduced from the discharge characteristics and assumed to be the same for charging.
- The capacity of the battery does not change with the amplitude of the current (no Peukert effect).
- The self-discharge of the battery is not represented.
- The battery has no memory effect.
- The voltage and the current can be influenced.

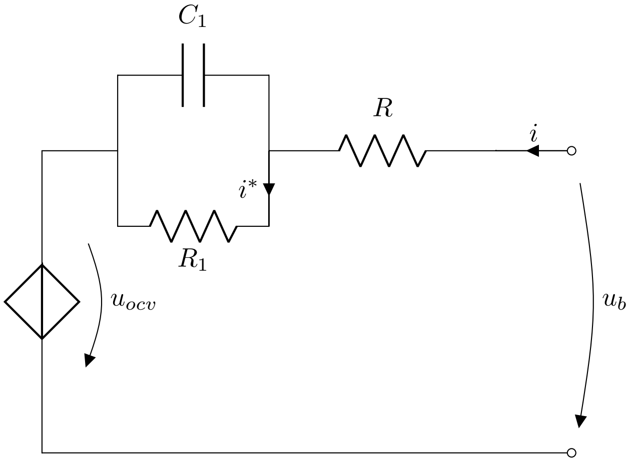

Figure 1: Equivalent circuit model of the battery

2 Basic equivalent circuit model

From the potential modeling methodologies the equivalent electrical circuit type was selected to create the basic battery model. The model was described in [2, 1]. The structure of the model can be seen in Figure 1. This model does not contain any temperature or aging effect.

2.1 Conservation balance equations

- The extracted capacity of the battery (q) can be described with the following equation (charge conservation):

$$\frac{d}{dt}q(t) = \frac{1}{3600}i(t) \tag{1}$$

The initial values of the extracted capacity are:

  - $q(t_0) = 0$, if the battery is fully charged and
  - $q(t_0) = Q$, if the battery is fully discharged.

The state of charge (SOC) of the battery (in percentages) can be computed as $(Q - q)/Q \cdot 100$.

- The low polarization current ($i^*(t)$) can be computed by applying a low-pass filter to the battery current i:

$$\frac{d}{dt}i^*(t) = -\frac{1}{\tau}i^*(t) + \frac{1}{\tau}i(t) \tag{2}$$

where $\tau = R_1C_1$ is the time constant of the RC circuit.

2.2 Constitutive equations

- The voltage of the internal resistance (R) can be expressed using Ohm's law:

$$u_r(t) = R \cdot i(t) \tag{3}$$

- The open circuit voltage is represented by a current controlled voltage source. Its voltage output depends on the current input: $u_{ocv} = f(i(t))$.

The open circuit voltage of the battery is a nonlinear function of the state of charge of the battery. The charge and discharge characteristics of the battery are usually different. The open circuit voltages ($u_{ocv}(t)$) during charging and discharging can be expressed with the following nonlinear functions controlling the voltage source:

$$u_{ocv}(t) = \begin{cases} E_0 - K \cdot \frac{Q}{q(t)+0.1Q} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)), & \text{if } i^*(t) < 0 \\ E_0 - K_r \cdot \frac{Q}{Q-q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)), & \text{if } i^*(t) \geq 0 \end{cases} \tag{4}$$

where:

- $q(t)$ is the extracted capacity (Ah)
- $i^*(t)$ is the polarization current corresponding to the diffusion voltage (A)
- $i(t)$ is the battery current (A)
- E_0 is the constant potential of the electrodes (V)
- K is the polarization coefficient (Ω)
- Q is the battery capacity (Ah)
- A is the exponential voltage (V)
- B is the exponential capacity (Ah^{-1})

The terms in the open circuit voltage equation have the following meanings:

- $K \cdot \frac{Q}{Q-q(t)} \cdot i^*(t)$ is the concentration polarization voltage
- $A\exp(-B \cdot q(t))$ is the exponential voltage that represents the initial voltage drop caused by the activation polarization

The output of the model is the battery voltage can be written using Kirchoff's voltage law:

$$u_b(t) = u_{ocv}(t) - u_r(t) \tag{5}$$

2.3 State space representation

Input variables:

- $i(t)$: battery current

State variables:

- $q(t)$: extracted charge of the battery
- $i^*(t)$: polarization current

Output variables:

- $u_b(t)$: battery voltage

State equations:

$$\frac{d}{dt}q(t) = \frac{1}{3600}i(t)$$
$$\frac{d}{dt}i^*(t) = -\frac{1}{\tau}i^*(t) + \frac{1}{\tau}i(t)$$

Output equations:

- Charge:

$$u_{b,ch}(t) = E_0 - K \cdot \frac{Q}{q(t) + 0.1Q} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R \cdot i(t)$$

- Discharge:

$$u_{b,d}(t) = E_0 - K \cdot \frac{Q}{Q - q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R \cdot i(t)$$

2.4 List of the model variables and parameters

2.5 Determination of the parameters

The battery parameters R and Q can be extracted from the datasheet of the examined battery. The parameters E_0, K, A, B can be determined from the nominal discharge curve of the battery usually provided by the manufacturer. The nominal discharge curve represent the battery voltage when discharging the battery with constant nominal current $i(t)$ [3]. The main regions of the discharge curve can be seen in Figure 2. The parameter B can be determined from the charge at the end of the exponential zone:

$$B = \frac{3}{Q_{exp}} \tag{6}$$

Table 1: Variables of the examined Li-ion battery

Variable	Name	Unit
$i(t)$	battery current	A
$u_b(t)$	battery voltage	V
$q(t)$	extracted capacity	Ah
$i^*(t)$	polarization current	A

Table 2: Parameters of the examined Li-ion battery

Parameter	Name	Unit	Nominal value	Temperature dependent	Age dependent
E_0	battery constant voltage	V	3.5784	+	-
R	internal resistance	Ω	0.014348	+	+
K	polarization coefficient	Ω	0.010749	+	-
Q	battery capacity	Ah	2.3	+	+
A	exponential zone amplitude	V	0.27712	-	-
B	exponential zone time constant inverse	$(\text{Ah})^{-1}$	26.5487	-	-
τ	time constant of the RC circuit	s	0.003	-	-

At the start of the discharging ($t = 0$) the extracted capacity ($q(0)$) is 0, and $i^*(0)$ is also 0. Therefore the fully charged battery voltage can be expressed as:

$$u_{full} = E_0 + A - R \cdot i(0) \tag{7}$$

At the end of the exponential zone ($t = t_{exp}$), the extracted capacity is $q(t_{exp}) = Q_{exp}$. Since the battery current is constant, $i(t) = i$, for all $t > 0$. The battery voltage at this point is the following:

$$u_{exp} = E_0 - K \cdot \frac{Q}{Q - Q_{exp}} \cdot i^*(t_{exp}) + A \cdot \exp(-\frac{3}{Q_{exp}} \cdot Q_{exp}) - R \cdot i(t_{exp}) \tag{8}$$

At the end of the nominal zone ($t = t_{nom}$) the extracted capacity is $q(t_{nom}) = Q_{nom}$. The battery voltage at this point is the following:

$$u_{nom} = E_0 - K \cdot \frac{Q}{Q - Q_{nom}} \cdot i^*(t_{nom}) + A \cdot \exp(-B \cdot Q_{nom}) - R \cdot i(t_{nom}) \tag{9}$$

The constant voltage (E_0), polarization coefficient(K) and the exponential zone amplitude (A) can be determined by solving the following system of linear equations:

$$u_{full} + R \cdot i(0) = E_0 - K \cdot 0 + A \tag{10}$$

$$u_{exp} + R \cdot i(t_{exp}) = E_0 - K \cdot \frac{Q}{Q - Q_{exp}} \cdot i^*(t_{exp}) + A \cdot exp(-3) \tag{11}$$

$$u_{nom} + R \cdot i(t_{nom}) = E_0 - K \cdot \frac{Q}{Q - Q_{nom}} \cdot i^*(t_{nom}) + A \cdot exp(-B \cdot Q_{nom}) \tag{12}$$

The parameter values of our examined Li-ion battery can be seen in Table 2.

3 Model with temperature effect

The operation of the battery is affected by the ambient and cell temperature.The rate of chemical reactions taking place in the battery are influenced by the temperature. For example at low temperatures diffusion decreases which results in a reduced capacity, or liquid electrolyte may freeze. At high temperatures unwanted chemical reactions and physical transformations may occur (corrosion, bubble formation etc.) which also lead to deteriorating performance and shortened lifetime. Internal impedance, self discharge and cycle life of the battery cell are also affected by the temperature. Within limits of operating temperature the performance usually improves with the increasing temperature. The effect of the temperature appears in the varying parameters of the battery such as the constant voltage (E_0), polarization coefficient (K), capacity (Q) and the internal resistance (R).

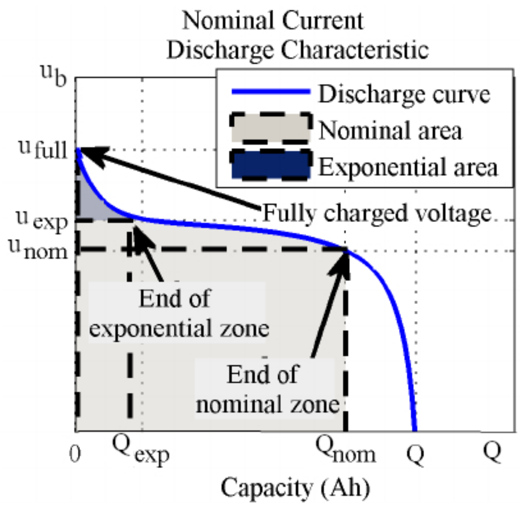

Figure 2: Typical nominal discharge characteristic of a battery [3]

3.1 Additional modelling assumptions

- The capacity depends on the ambient temperature (T_a).
- The constant voltage, the polarization coefficient, the polarization resistance and the internal resistance depend on the internal (cell) temperature of the battery.
- The form of the charge and discharge equations remain unchanged.

3.2 Additional constitutive equations

- The change of polarization coefficient and internal resistance with the temperature can be derived from the Arrhenius law:

$$K(T) = K|_{T_{ref}} \cdot \exp\left(\alpha\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \tag{13}$$

$$R(T) = R|_{T_{ref}} \cdot \exp\left(\beta\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \tag{14}$$

- The temperature dependency of the capacity and the constant voltage can be written in the following form:

$$Q(T_a) = Q|_{T_{ref}} + \frac{\Delta Q}{\Delta T} \cdot (T_a - T_{ref}) \tag{15}$$

$$E_0(T) = E_0|_{T_{ref}} + \frac{\partial E}{\partial T}(T - T_{ref}) \tag{16}$$

where

  - T_{ref} is the nominal ambient temperature (K)
  - T is the internal or cell temperature of the battery (K)
  - T_a is the ambient temperature (K)
  - α is the Arrhenius rate constant for the polarization coefficient (K)
  - β is the Arrhenius rate constant for the internal resistance
  - $\Delta Q/\Delta T$ is the maximum capacity temperature coefficient (Ah/K)
  - $\partial E/\partial T$ is the reversible voltage temperature coefficient (V/K)

- Substituting these temperature dependent parameters into Eq. (4) we get the temperature dependent open circuit voltage equations:

$$u_{ocv}(t, T, T_a) = \begin{cases} \text{if } i^*(t) < 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{q(t)+0.1Q(T_a)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) \\ \text{if } i^*(t) \geq 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{Q(T_a)-q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) \end{cases} \tag{17}$$

- The output equation can be written as the difference between the open circuit voltage and the voltage drop of the internal resistance:

$$u_b(t, T, T_a) = u_{ocv}(t, T, T_a) - R(T) \cdot i(t)$$

which has the following form in case of charging and discharging:

$$u_b(t, T, T_a) = \begin{cases} \text{if } i^*(t) < 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{q(t)+0.1Q(T_a)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R(T) \cdot i(t), \\ \text{if } i^*(t) \geq 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{Q(T_a)-q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R(T) \cdot i(t) \end{cases} \quad (18)$$

3.3 Additional balance equations

- The internal energy balance equation of the battery:
The internal temperature of the battery at a time t is computed from its energy balance equation as:

$$C_p \frac{dT}{dt} = \kappa(T_a - T) + \kappa R_{th} P_{loss} \quad (19)$$

where

  - C_p is the heat capacity of the battery material (J/K)
  - κ is the heat transfer coefficient, cell to ambient (W/K)
  - R_{th} is the thermal resistance, cell to ambient (K/W)
  - $t_c = \frac{C_p}{\kappa}$ is the thermal time constant, cell to ambient (s)
  - P_{loss} is the overall heat generated (W) during the charge/discharge process:

$$P_{loss} = (E_0(T) - u_b) \cdot i + \frac{\partial E}{\partial T} \cdot i \cdot T \quad (20)$$

  - $\partial E/\partial T \cdot i \cdot T$ is the entropic heat

From the above equation we get the state equation of the temperature as a state variable:

$$\frac{d}{dt}T(t) = \frac{1}{t_c}(T_a - T(t)) + \frac{1}{t_c} \cdot (P_{loss} \cdot R_{th}) \quad (21)$$

Substituting P_{loss} with Equation (20) and u_b with Equation (22) we get the state equations of the internal temperature:

$$\frac{d}{dt}T(t) = \begin{cases} \text{if } i^*(t) < 0: \\ -\frac{1}{t_c}T(t) + \frac{R_{th}}{t_c} \cdot \Big(K(T) \cdot \frac{Q(T_a)}{q(t)+0.1 \cdot Q(T_a)} \cdot i^*(t) \cdot i(t) - A\exp(-B \cdot q(t)) \cdot i(t) + \frac{\partial E}{\partial T} \cdot i(t) \cdot T\Big) + \frac{T_a}{t_c} \\ \text{if } i^*(t) \geq 0: \\ -\frac{1}{t_c}T(t) + \frac{R_{th}}{t_c} \cdot \Big(K(T) \cdot \frac{Q(T_a)}{Q(T_a)-q(t)} \cdot i^*(t) \cdot i(t) - A\exp(-B \cdot q(t)) \cdot i + \frac{\partial E}{\partial T} \cdot i \cdot T\Big) + \frac{T_a}{t_c} \end{cases} \quad (22)$$

3.4 Parameter varying model

Input variables:

- $i(t)$: battery current

State variables:

- $q(t)$: e charge of the battery
- $i^*(t)$: polarization current
- T: internal temperature of the battery

Output variables:

- $u_b(t)$: battery voltage

State equations:

$$\frac{d}{dt}q(t) = \frac{1}{3600}i(t)$$
$$\frac{d}{dt}i^*(t) = -\frac{1}{\tau}i^*(t) + \frac{1}{\tau}i(t)$$

$$\frac{d}{dt}T(t) = \begin{cases} \text{if } i^*(t) < 0: \\ -\frac{1}{t_c}T(t) + \frac{R_{th}}{t_c} \cdot \left(K(T) \cdot \frac{Q(T_a)}{q(t)+0.1 \cdot Q(T_a)} \cdot i^*(t) \cdot i(t) - A\exp(-B \cdot q(t)) \cdot i + \frac{\partial E}{\partial T} \cdot i(t) \cdot T\right) + \frac{T_a}{t_c} \\ \text{if } i^*(t) \geq 0: \\ -\frac{1}{t_c}T(t) + \frac{R_{th}}{t_c} \cdot \left(K(T) \cdot \frac{Q(T_a)}{Q(T_a)-q(t)} \cdot i^*(t) \cdot i(t) - A\exp(-B \cdot q) \cdot i(t) + \frac{\partial E}{\partial T} \cdot i(t) \cdot T\right) + \frac{T_a}{t_c} \end{cases} \tag{23}$$

Output equation:

$$u_b(t, T, T_a) = \begin{cases} \text{if } i^*(t) < 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{q(t)+0.1Q(T_a)} \cdot i^*(t) + A \cdot \exp(-B \cdot q) - R(T) \cdot i, \\ \text{if } i^*(t) \geq 0: \\ E_0(T) - K(T) \cdot \frac{Q(T_a)}{Q(T_a)-q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R(T) \cdot i(t) \end{cases} \tag{24}$$

3.5 List of the model variables and parameters

The variables and the parameters of the temperature dependent battery model can be seen in Table 3. and Table 4.

Table 3: Variables of the examined Li-ion battery

Variable	Name	Unit
$i(t)$	battery current	A
$u_b(t)$	battery voltage	V
$q(t)$	extracted capacity	Ah
$i^*(t)$	polarization current	A
$T(t)$	internal temperature	K

Table 4: Parameters of the examined Li-ion battery

Parameter	Name	Unit	Nominal value
$E_0(T_{ref})$	battery constant voltage at nominal ambient temperature	V	3.4265
$R(T_{ref})$	internal resistance at nominal ambient temperature	Ω	0.014
$K(T_{ref})$	polarization coefficient at nominal ambient temperature	Ω	$6.4489e-4$
$Q(T_{ref})$	battery capacity at nominal ambient temperature	Ah	2.3
A	exponential zone amplitude	V	0.3802
B	exponential zone time constant inverse	$(\text{Ah})^{-1}$	26.5487
τ	time constant of the filter	s	0.003
T_a	ambient temperature	K	-
T_{ref}	nominal ambient temperature	K	298.15
α	Arrhenius rate constant for the polarization coefficient	K	1901.9
β	Arrhenius rate constant for the internal resistance	K	9058.7
$\Delta Q/\Delta T$	maximum capacity temperature coefficient	Ah/K	0.0037
$\partial E/\partial T$	reversible voltage temperature coefficient	V/K	$1.1927e-5$
R_{th}	thermal resistance	K/W	0.6
t_c	thermal time constant	s	1000

4 Model with aging effect

It is well-known that the performance of the battery slowly degrades with the usage. The age of the battery is usually measured with the number of charge-discharge cycles. The aging process is affected by many factors, such as cycle number, depth of discharge, temperature, current rates, resting time between cycles etc. In this section a simple empirical model is introduced, that describe the most significant changes in parameters.

4.1 Additional modelling assumptions

- The internal resistance (R) and the battery capacity (Q) are the two parameters, that are affected by the aging.
- The only factor, that affect the aging is the cycle number.
- The model equations apply to the nominal ambient temperature.

4.2 Additional constitutive equations

In this aging model, empirical relationships are used to describe the change of the internal resistance and the capacity with respect to cycle numbers.

- The internal resistance is increasing with the cycle number. The following equation describes the relationship between the battery internal resistance (R) and the cycle number (n):

$$R(n) = a \cdot exp(b \cdot n) + c \cdot exp(d \cdot n) \tag{25}$$

- The capacity of the battery is decreasing with the cycle number. The relationship between the capacity (Q) and the cycle number (n) is linear:

$$Q(n) = e \cdot n + f \tag{26}$$

The nominal parameter values related to the aging of the examined Li-ion battery can be seen in Table 5.

Table 5: Parameter values related to the aging of the examined Li-ion battery

Parameter	Value
a	0.01525
b	3.333 e-5
c	3.246 e-5
d	6.791 e-4
e	-2.085 e-4
f	2.425

4.3 State space representation

The state space representation of the age-dependent battery model differs from the basic model (Section 2.3) only in the output equations.

Input variables:

- $i(t)$: battery current

State variables:

- $q(t)$: extracted charge of the battery
- $i^*(t)$: polarization current

Output variables:

- $u_b(t, n)$: battery voltage

State equations:

$$\frac{d}{dt}q(t) = \frac{1}{3600}i(t)$$
$$\frac{d}{dt}i^*(t) = -\frac{1}{\tau}i^*(t) + \frac{1}{\tau}i(t)$$

Output equations:

- Charge:

$$u_{b,ch}(t,n) = E_0 - K \cdot \frac{Q(n)}{q(t) + 0.1Q(n)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R(n) \cdot i(t)$$

- Discharge:

$$u_{b,d}(t,n) = E_0 - K \cdot \frac{Q(n)}{Q(n) - q(t)} \cdot i^*(t) + A \cdot \exp(-B \cdot q(t)) - R(n) \cdot i(t)$$

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