Randles Circuit Parameters Set Up for Battery Simulations in LS-DYNA®

Sarah Bateau-Meyer[1], Pierre L'Eplattenier[1], Jie Deng[2], Min Zhu[2], Chulheung Bae[2], Theodore Miller[2]

[1]*Livermore Software Technology Corporation, Livermore, CA*
[2]*Ford Motor Company, Research and Innovation Center, Dearborn, MI*

Abstract

A multi physics model for battery abuse was recently introduced in LS-DYNA. This model predicts coupled mechanical, thermal, electrical and electro-chemical responses. The complex electro-chemical behavior is described by simple equivalent circuits, called "Randles" circuits.
Each Randles circuit connects two vis-à-vis nodes of the positive and negative current collector layers and consists in a State-Of-Charge (SOC) dependent voltage source, an internal resistance and a resistance-capacitance (RC) loop. The choice of the values of the circuit components in the LS-DYNA cards is let to the user and strongly depends on the battery cell. This paper thus proposes a procedure to choose with precision the Randles circuit components values from simple voltage and current measurements on the cell. The parametrization process is done by a parameter identification on these experimental coupled voltage/current measurements, such as Hybrid Pulse Power Characterization (HPPC) test results, in a single Randles circuit, representing the whole cell.
The paper will present briefly the distributed Randles circuit model and the experimental tests before exposing one parameter identification method.

1- Introduction

Following the increasing demands, LSTC introduced in 2017 the Randles circuit model into the LS-DYNA electromagnetic solver to simulate the complex electrochemistry happening in the layers of Lithium-ion batteries. A Lithium-ion battery is a rechargeable battery in which lithium ions move from the negative electrode to the positive electrode during its discharge into a load, and back when charging. The current flow as well as the heat that it generates are modeled by the equivalent Randles circuit. It has been introduced in Ref. [1], paper published for the 14th International LS-DYNA Users Conference. A reminder of such circuit is given in section 2.

The choice of the parameters of the Randles circuit model is primordial as they entirely characterize the battery electrochemical properties. During the setup of a battery simulation using LS-DYNA, the user must fill up a particular keyword to define the Randles circuit model. It may be *EM_ BATTERY_RANDLES if the battery layers are built with solid elements, *EM_RANDLES_LAYERED if the layers are made of composite tshell elements, and in particular cases where the cell does not need to be represented, *EM_RANDLES_MESHLESS. The present paper has the objective of guiding every LS-DYNA user in the evaluation of the keyword parameters.

The parametrization process consists in the comparison of experimental results known by the user with results given by an analytical solution. The analytical solution parameters are tuned by an optimization algorithm so that the analytical results match the experimental ones. Section 3 gives an overview of the experimental tests characterizing a battery whereas section 4 provides the analytical solution and the processes to optimize the Randles circuit parameters regarding the experiments. A Matlab program performs the entire parametrization process and is quoted in section 4. The users are invited to download it and take advantage of it as a starting base. The experimental results used all along the present paper have been provided by the Ford team.

2- The Electrothermal Randles Circuit Model in LS-DYNA

2-1 The Distributed Randles Model

To simulate the electrochemistry happening in the layers of a unit cell, a Randles circuit is built between each vis-à-vis nodes of the positive and negative current collectors as shown on the figure 1. A Randles circuit consists of an ideal voltage - called also Open Circuit Voltage (OCV) - source, an internal resistance and n parallel RC circuits, n being the order of the model. As a consequence, a Randles circuit having only one RC loop is said of 1st order. It has been proved that the presence of a unique RC loop is enough to accurately model the damping effects present in the measured voltage. The circuit components depend on the State of Charge (SOC), the temperature and the current direction. The OCV source is assumed to only depend on the SOC.
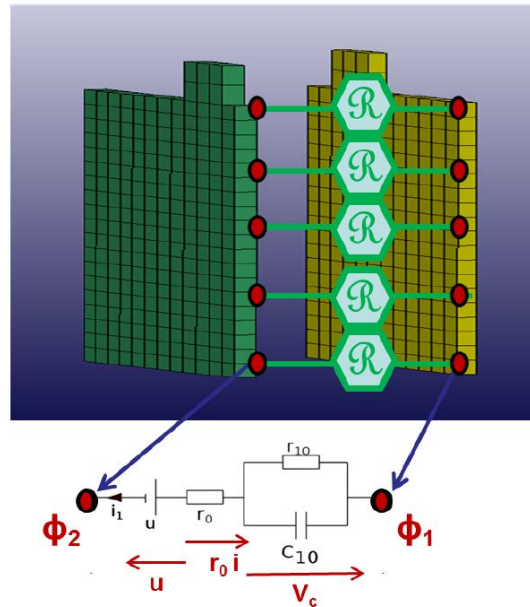

Figure 1: Schematic for a distributed Randles circuit between the two current collectors

If k is the number of nodes of one current collector face, the model includes k 1st order Randles circuits. They are equivalent to the so-called 0-D Randles circuit shown on the figure 2 with:

$$R0 = k * r0$$
$$R10 = k * r10$$
$$C10 = c10/k$$

(1)

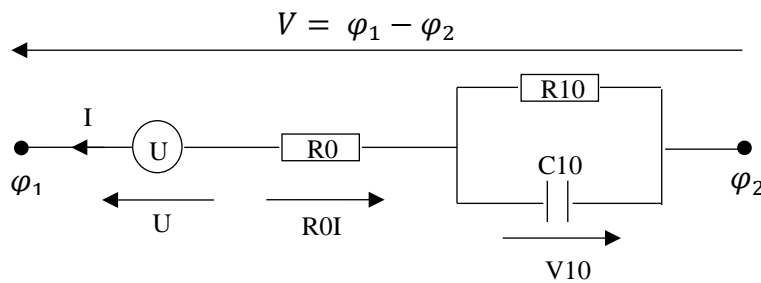*Figure 2: a 0-D Randles circuit, in a discharge position*

The total voltage across the electrodes is given by:

$$V = U + R0I + V10 \text{ for a charge}$$
$$V = U - R0I - V10 \text{ for a discharge}$$

(2)

With:

$$\frac{dV10}{dt} = \frac{I}{C10} - \frac{V10}{R10C10}$$

(3)

2-2 LS-DYNA Keywords

The LS-DYNA Keyword User's Manual Volume III presents three different keywords to define the distributed Randles circuit parameters.

*EM_BATTERY_RANDLES must be used with a solid mesh. It distinguishes by the parameters CPPPART, CCNPART, SEPPART, PELPART and NELPART that represent the identities respectively of the positive and negative current collectors, the separator and the positive and negative electrodes solid parts.

*EM_RANDLES_LAYERED must be used with a mesh composed of composite tshell elements. It distinguishes by the parameter PSID that represents the part set identity of all the composite tshell parts of the battery. The layers of each of these parts are defined inside the keyword *PART_COMPOSITE_TSHELL.

*EM_RANDLES_MESHLESS must be used to define a lumped Randles circuit therefore not associated to any mesh.

The rest of the parameters are common to the three keywords. They are listed and defined below.

➢ RDLID
  is the identity of the defined Randles battery.

➢ RDLTYPE
  is the type of the Randles battery. Note that, at this date, only the pouch type is available: well in fact the cylindrical also.

➢ RDLAREA
  Determines the parameters scaling method. By default, the parameters are defined for the whole cell and will be automatically scaled in each Randles circuit like in equation (1).

➢ Q
  is the cell capacity.

➢ CQ
  is the SOC conversion factor (%/s). It is linked to the cell capacity q by:

$$q = \frac{Q}{cQ} * SOC$$

(4)

If Q has been defined in Ah whereas q is internally defined in the Coulombs SI unit, we have:

$$q = Q * 3600 * \frac{SOC}{100}$$

(5)

Hence $cQ = \frac{1}{36}$

➢ SOCINIT

is the initial SOC of the battery.

➢ SOCTOU

gives the value of the OCV source U. It may be a constant value if the parameter is written positively, or otherwise the load curve identity giving the value of U as a function of the SOC. The determination of such a curve is detailed in section 4-1.

➢ R0CHA/R10CHA/C10CHA

give the values of the circuit components R0, R10 and C10 when the current flows in the charge direction. It may be a constant value if the parameter has a positive value, or otherwise the load curve or table identity giving the value of the component as a function of the SOC. A table gives the component value versus SOC for different temperatures. The determination of such functions is detailed in section 4-2.

➢ R0DIS/R10DIS/C10DIS

give the values of the circuit components R0, R10 and C10 when the current flows in the discharge direction. The definition is similar as the R0CHA/R10CHA/C10CHA one.

➢ TEMP

is the constant temperature value used for the parameters if the thermal solver is not activated. The activation is managed by the keyword FRTHERM.

➢ FRTHERM

determines if the temperature used for the parameters is the constant TEMP or the one actuated by the thermal solver.

➢ R0TOTHERM

determines if the Joule heating created by the internal resistance R0 is added or not to the thermal solver.

➢ DUDT

gives the value of the term $\frac{dU}{dT}$ in function of the SOC. It is needed in the calculation of the reversible heat that may be added, additionally with the Joule heating, to the thermal solver.
This heat is linked to the entropic change of electrode reactions.

➢ TEMPU

sets the temperature unit used in the Randles circuit thermal parameters definition.

➢ USESOCS

activates the use of the damped term SOC shift which satisfies the equation:

$$\frac{d(SOCshift)}{dt} + \frac{SOCshift}{\tau} = \frac{f(I,T)}{\tau} \tag{6}$$

The SOC shift may be added to model the diffusion limitations occurring at sustained high rate discharges. It is relevant in scenarios such as external short or overcharge.

➢ TAUSOCS
is the damping time τ in equation (6)

➢ SOCSLCID
gives the load curve $f(i)$ of equation (6)
The determination of TAUSOCS and SOCSLCID is detailed in section 4-3.

3- Overview of the Characteristic Experimental Tests

3-1 C/10 Capacity Charge and Discharge Tests

A XC charge/discharge capacity test is the voltage V measurement for the time the cell is being charged /discharged. The applied current is constant and chosen such as the charge/discharge time be of 1/X hours.

The determination of the parameter SOCTOU is done via C/10 capacity tests. A current rate allowing the charge/discharge of the cell capacity in a time of ten hours is applied to the cell. The current rate and the measured voltage during the typical experimentation are shown on the figure 3. The experiment temperature is the 25°C room temperature.
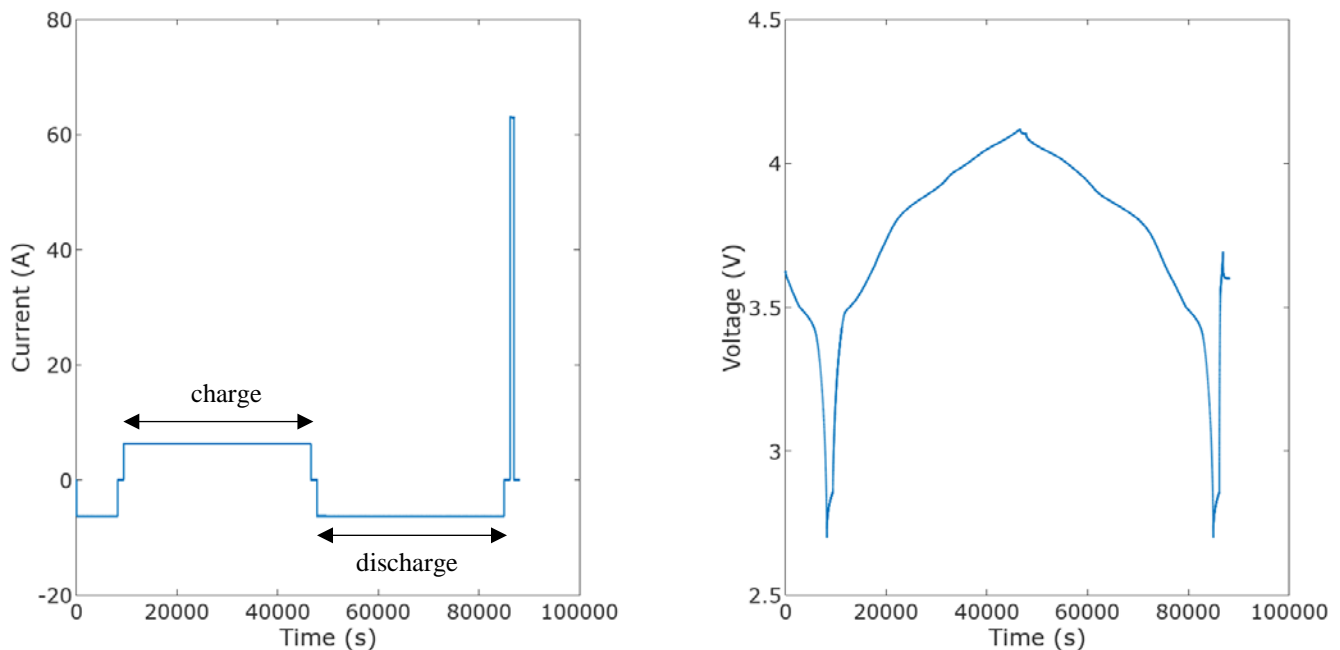

Figure 3: C/10 capacity test example, for a type E cell at 25°C

In comparison to ten hours, the circuit components dynamic is negligible. As a consequence, from (2), the measured voltage is directly equal to the OCV.

3-2 Hybrid Pulse Power Characterization (HPPC) Test

A HPPC test is the voltage V measurement of the cell following a series of 10 s charge and discharge pulses, at different discrete SOCs and a given temperature. The profile of a HPPC test is given by the figure 4.
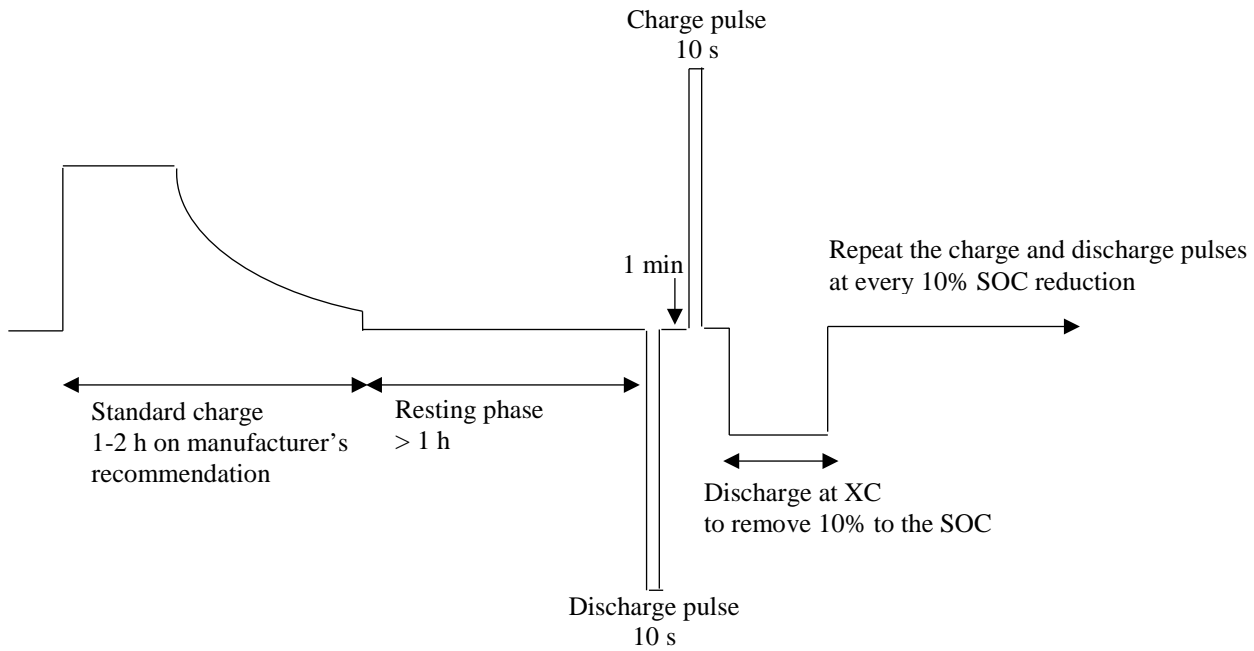
Figure 4: HPPC test profile – Current (A) in function of time

During a pulse the cell does not have the time to discharge and the SOC hence the OCV stay constant. The model components R0, R10 and C10 may thus be defined from (2), at each discrete SOC, and separately for the charge and the discharge.

Practically the SOCs vary from 90% to 10% by increments of 10%. The test results for the entire 9 SOCs are given by the figure 5.
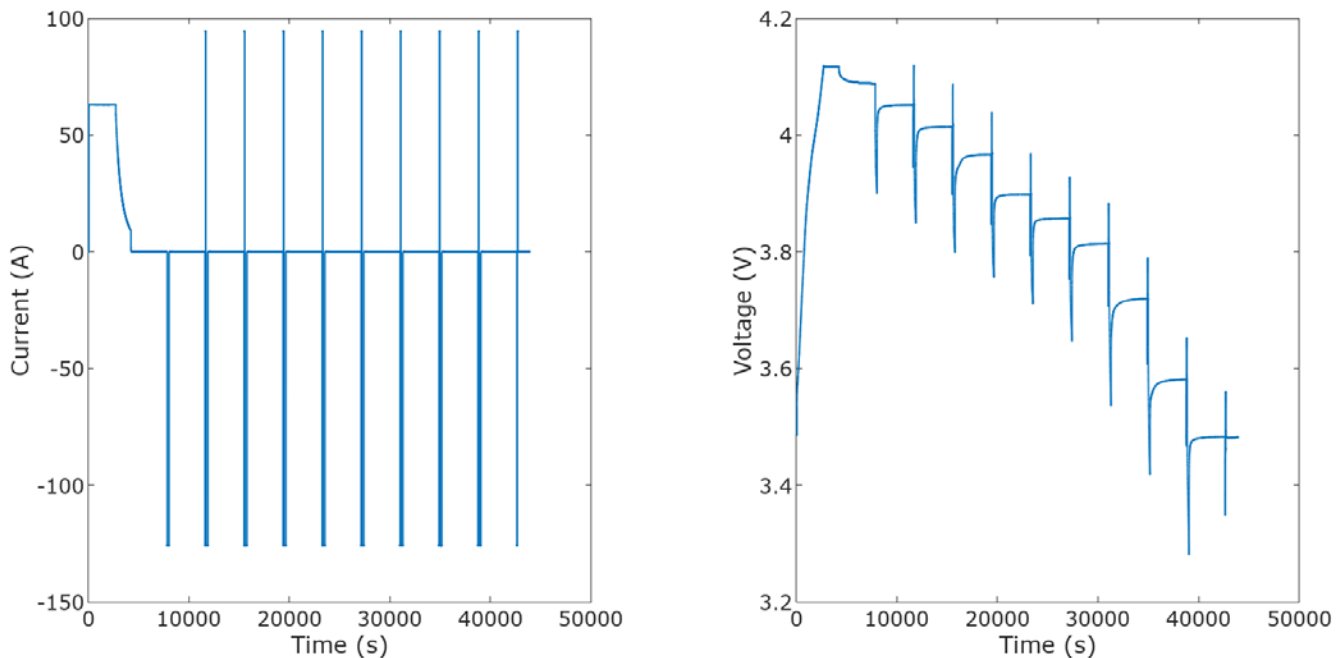

Figure 5: HPPC test example, for a type E cell at 25°C
The current profile indicates that the cell is first fully charged and is then subject to a discharge removing 10% of the SOC. Follows 9 charge and discharge pulses, each sequences being separated by the 10% SOC discharge.

A HPPC test should be conducted for different battery cell operating temperature.

3-3 Multi-Rate Capacity Discharge Test

A multi-rate capacity discharge test is the succession of capacity discharges for different C-rates – see 3-1. The cell is fully charged between each discharge with an adequate time. Figure 6 shows an example of such a test, conducted with C-rates of 1,2,3 and 4.
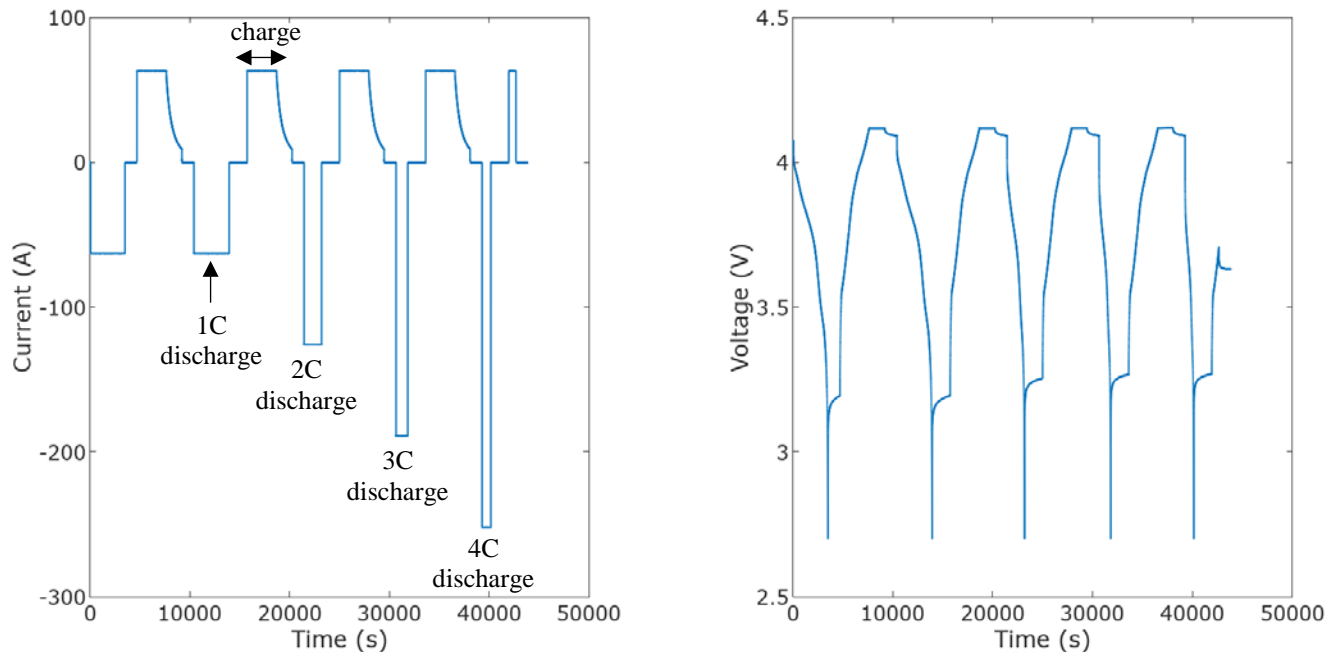

Figure 6: Multi-rate capacity test example, for a type E cell at 25°C

To parameterize the additional term SOC shift the test must be conducted with high C-rates as 5 or 10.

4- Parametrization Process

With the previous experimental results, one can determine the Randles battery parameters SOCTOU, R0, R10, C10 and if needed the SOC shift terms TAUSOCS and SOCSLCID. The present part proposes one method allowing to get easily and with a good accuracy these parameters. This method has been applied in the Matlab program presented in the Appendix A.

4-1 SOCTOU Parameter

SOCTOU is determined using the experimental results from the C/10 capacity test detailed in 3-1.
In the Matlab program the following is executed by the function *getOCV*.

➢ Calculation of the SOC using the equations (4) and (5)
For every measures *n:*

$$q(n + 1) = q(n) + I(n) * (t(n) - t0)$$
$$SOC(n + 1) = cQ * q(n + 1)/Q$$

(7)

With t the time at the measure n and $t0$ the initial charge/discharge time.
Note that I, the applied current, is positive for a charge and negative for a discharge . The initial charge should be 0 or Q, expressed in Coulombs, depending if the battery is charging or discharging.

➢ Expression of the measured charge and discharge voltages in terms of SOC

Two curves are obtained: on one hand the charge voltage in function of the increasing SOC and on the other hand the discharge voltage in function of the decreasing SOC. A linear interpolation allows to get the same number of points between the two curves. In the Matlab program we chose to interpolate the voltages for SOCs going from 0 to 100 with a step of 0.01.

➢ Calculation of the OCV (= U)
The OCV is taken as the average of the charge and discharges curves following:

$$OCV = \frac{V_{charge\_interp} + V_{discharge\_interp}}{2} \tag{8}$$

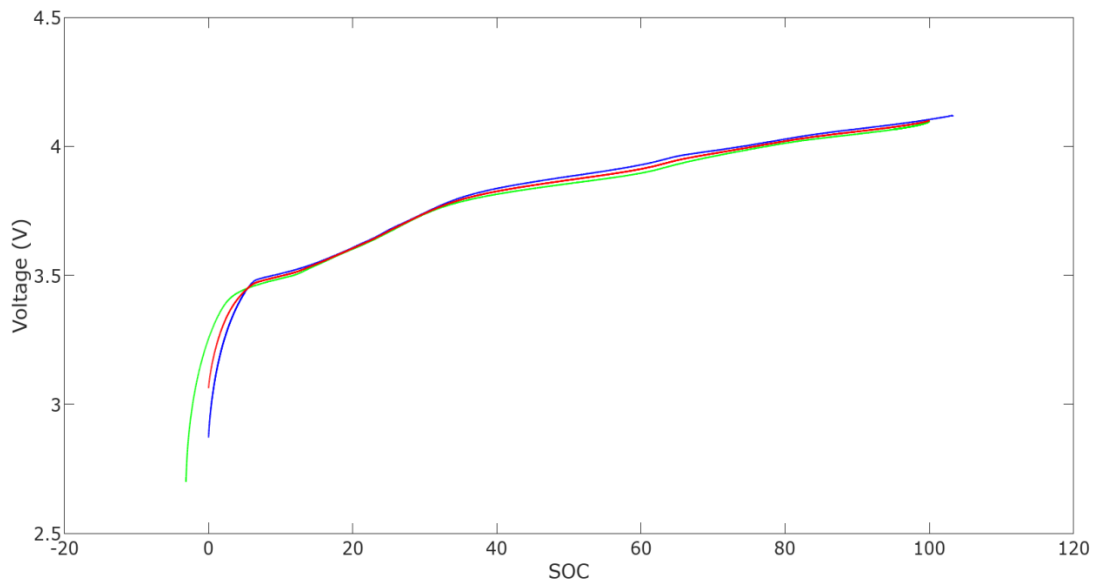The discharge, charge and OCV curves are shown on the figure 7.

Figure 7: Voltages in function of the SOC - in blue: during the charge, in green: during the discharge – and in red: OCV taken as the average of the discharge and charge curves

In the Matlab program we registered the SOC and its associated OCV in a 2 columns matrix SOCTOU. The matrix should be saved and rewritten under the *DEFINE_CURVE keyword defining the battery parameter SOCTOU.
In the following any OCV is determined by interpolation knowing the SOC or the opposite.

In the load curve, it is recommended to extend OCV for SOC values slightly inferior to 0 and superior 100.

4-2 Resistance and Capacitance Parameters

The resistance and capacitance parameters are determined using the experimental results from the HPPC test detailed in 3-2.
In the Matlab program the following is executed by the function *getComponents*.

The profile of a test result voltage at one discrete SOC is shown on the figure 8. Remarkable points are represented.
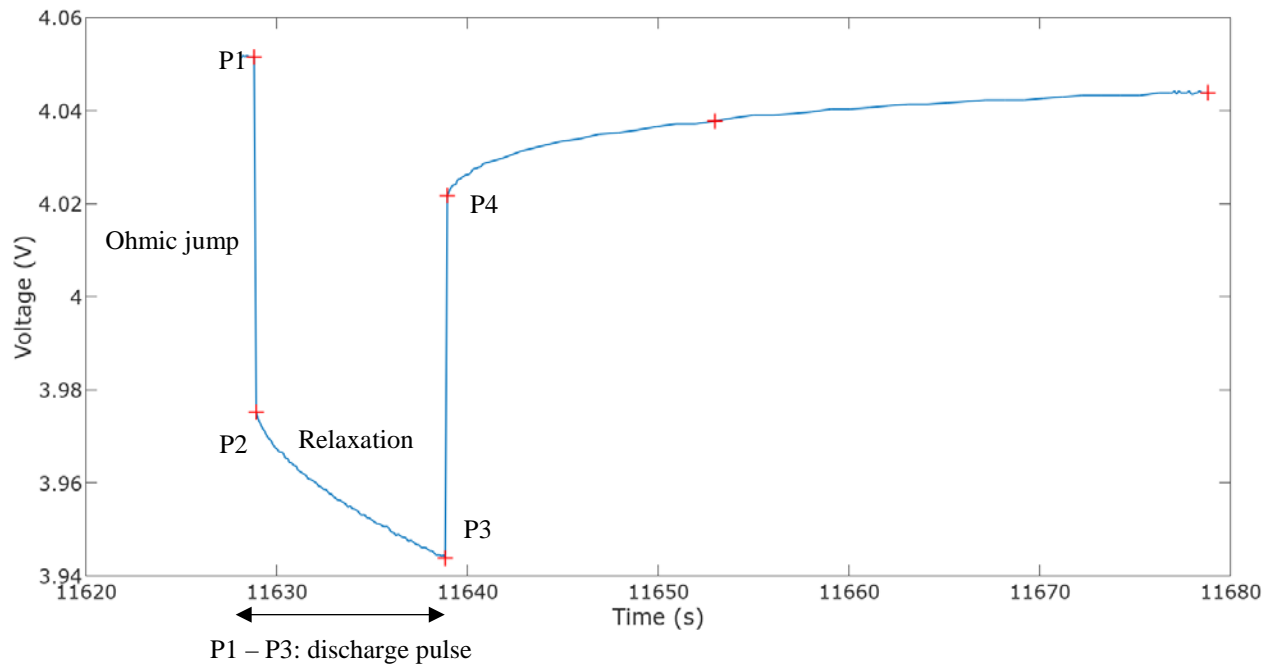

Figure 8: HPPC test measured voltage profile, for a pulse at 90% SOC, at 25°C

4-2-1 The resistance R0

The resistance R0 captures the initial ohmic voltage jump following a step change in the current. Ohm's law gives:

$$R0 = \frac{|V(P4) - V(P3)|}{|I(P4) - I(P3)|}$$
$$\leftrightarrow \quad R0 = \frac{|V(P2) - V(P1)|}{|I(P2) - I(P1)|}$$

(9)

4-2-2 The parallel R10 and C10 pair

R10 and C10 capture the relaxation period following the application or removal of the current. They are identified using a linear least squares algorithm to fit the experimental results. The next steps must be repeated for each discharge and charge pulses.

➢ For each measure n inside the relaxation period of a given pulse:

- Calculation of the SOC using (7)
  The initial charge q is chosen such as $U(1) = V(P1)$.

- Deduction of U

- Calculation of the potential difference between the R10 and C10 pair
  (2) gives:
  $$V10 = -U + V - R0I \text{ for a charge}$$
  $$V10 = U - V - R0I \text{ for a discharge}$$

(10)

With I the absolute value of the applied current and V the measured voltage

- Calculation of $\frac{dV10}{dt}$

➢ The circuit equation (3) can be rewritten under the matrix form:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ \vdots & \vdots \\ a_{N1} & a_{N2} \end{bmatrix} \begin{bmatrix} \dfrac{1}{R10C10} \\ \dfrac{1}{C10} \end{bmatrix} \quad \leftrightarrow \quad Y = A\theta \tag{11}$$

With $y_n = \frac{dV10}{dt}(n)$, $a_{n1} = -V10(n)$, $a_{n2} = I(n)$

The approximate solution of the linear system (11) is:
$$\theta = (A^T A)^{-1} A^T y \tag{12}$$

- Solving of the linear system with the Matlab function *ols*

- Deduction of C10 then R10

➢ For comparison the theoretical voltage may be calculated as followed:

- Calculation of $V10$
  (3) gives:

$$V10(n+1) = V10(n) + \big(t(n+1) - t(n)\big)\big(\frac{I(n)}{C10} - \frac{V10(n)}{R10C10}\big) \tag{13}$$

  With an initial V10 equal to 0.

- Calculation of the theoretical voltage using (2)

Figure 9 shows the analytical voltage determined with the optimized R10 and C10 for the discharge pulse at 90% SOC.
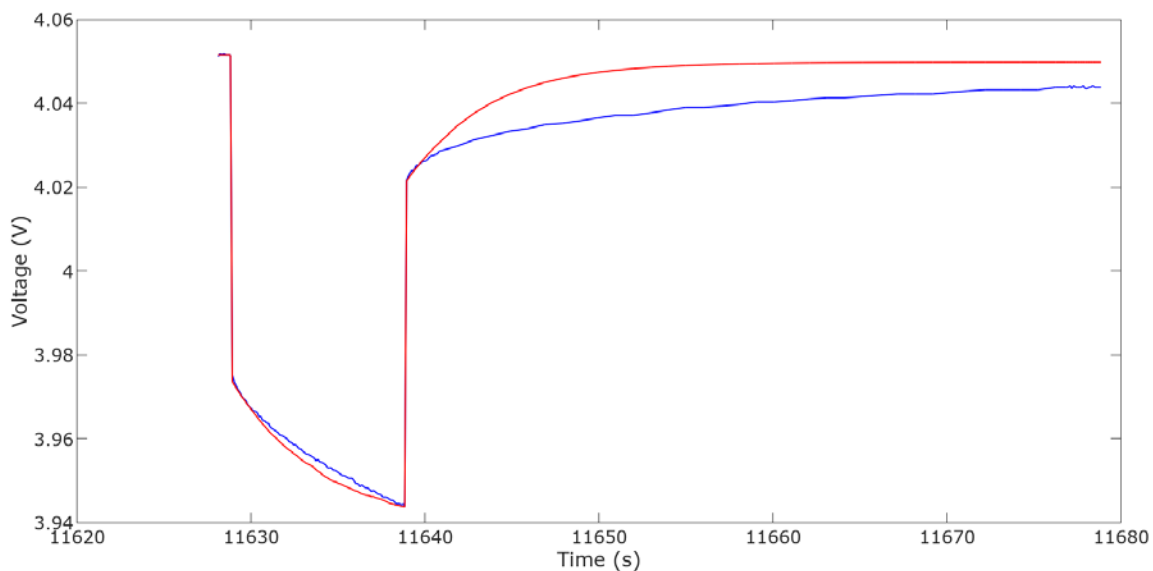

Figure 9: Comparison of the experimental (in blue) and analytical (in red) voltage profiles for a discharge pulse at 90% SOC, at 25°C

In the Matlab program we registered the components values in 2 columns matrix such as R0_D. R0_D gives the value of the component R0, in a discharge situation, for a given SOC. The SOCs are going from 10 to 90 with a step of 10 but should be extended manually. The procedure must be repeated for different battery cell operating temperatures. All the matrix should be saved and rewritten under *DEFINE_TABLE keywords giving the components parameters values in function of the temperature and the SOC.

Part 4-1 and 4-2 gave the parametrization process of the 0-D Randles circuit components U, R0, R10 and C10. Therefore, the components have been defined for the whole battery cell. If the battery parameter RDLAREA is equal to 2 the components values will be automatically scaled in each Randles circuit. Otherwise the conversion should be done manually.

4-3 SOC Shift Parameters

At high rate discharges the Randles battery model studied may not be enough to model the behavior of a battery. The following picture shows the voltage profile during discharges of different C-rates for a type A cell.
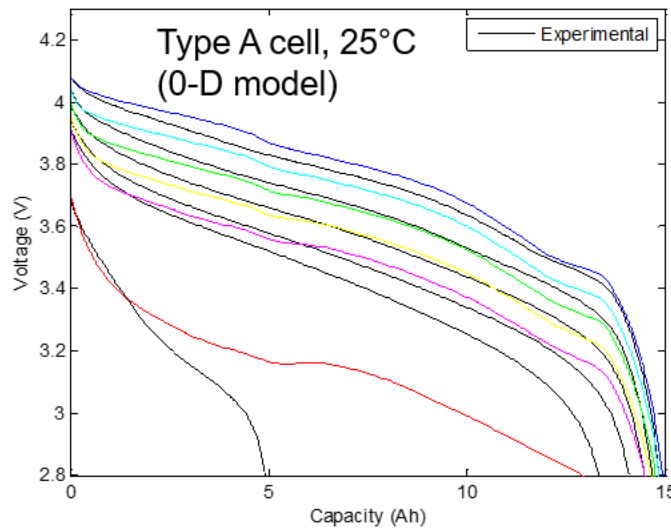

Figure 10: Comparison of the experimental (in black) and analytical (in color) voltage profiles for discharge pulses at C-rates of 1C, 2C, 3C, 4C, 5C and 10C for a type A cell at 25°C

The discharges at C-rates of 5C and 10C cannot, in this example, be correctly modeled by the usual Randles battery model. A SOC shift term may be added to the SOC term to reevaluate the voltage source U and the internal resistance R0, taking thus into account the diffusion limitations occurring at the high rate discharges. The amended model is represented by the figure 11.
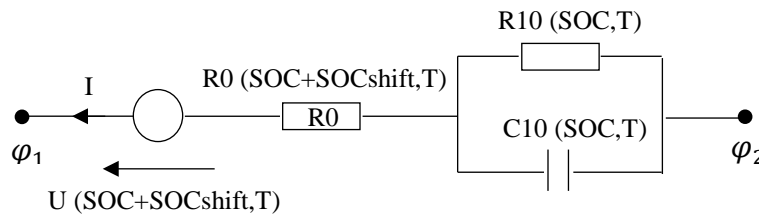

Figure 11: Amended Randles battery model for high rate discharges

The SOC shift is a damped term that satisfies the equation (6). We propose in this part a method to determine the terms τ and $f(I, T)$.

$f(I,T)$ is optimized for each discharge capacity test, at given current I and temperature T, and τ is optimized over all the tests. f optimization is made by the Matlab function *fminsearch*. The general procedure is explained below.

For every τ – e.g. going from 40 to 800 with a step of 10:

➢ For every discharge capacity test, at given I and T:

- Calculation of the SOC for every measures n similarly to (7)
  Working with the absolute value of the applied current in the Matlab program, we modified in the equation (7) the sign + for a –.

- Calculation of the SOC shift
  (6) gives:

$$SOCshift(n+1) = SOCshift(n) - \big(t(n+1) - t(n)\big)\Big(\frac{SOCshift(n)}{\tau} - \frac{f}{\tau}\Big) \qquad (14)$$

  Where f value is given by the function *fminsearch*.

- Deduction of SOCshifted such as:
$$SOCshifted = SOC + SOCshift$$

- From SOCshifted deduction of U, R0, R10 and C10

- Calculation of V10 and then the theoretical voltage Vth

- Calculation of the Root Mean Square Error (RMSE) using:

$$J(I) = w_1 \sqrt{\frac{1}{N}\sum_n (Vth(n) - Vexp(n))^2} + w_2|Vth(N) - Vexp(N)| \qquad (15)$$

Where N is the total number of measures, $Vexp$ is the measured voltage, and w_1 and w_2 are the weights given to each term, to the RMSE and the lower limit voltage error (e.g. 1 and 2).

The aim of all the previous steps is to determine the parameter f that minimizes J. J is therefore the objective function of *fminsearch* and f the searched parameter. It exists one J per discharge capacity test.

➢ Summation S of every J

The chosen τ is the one minimizing S. It corresponds to the Randles battery parameter TAUSOCS.
f should be saved and rewritten under a *DEFINE_TABLE keyword giving its value in function of the temperature and the current and associated to the Randles battery parameter SOCSLCID.

In the Matlab program the two parameters are determined using the experimental results from the multi-rate discharge capacity test detailed in 3-3. The execution is made by the function *getSocShift*. Note that our discharge capacity tests have been made at C-rates of 1C, 2C, 3C and 4C which are usually too low to capture the diffusion limitation phenomenon clearly. As a result, the usual Randles battery model is accurate enough to model the cell subject to these discharges and the SOC shift calculated at each measure n is close to 0. Figure 12

compares the voltage during the discharges on our type E cell at 25°C to the analytical voltage determined without shifted SOC. With the additional SOC shift term the voltage profile is almost identical.
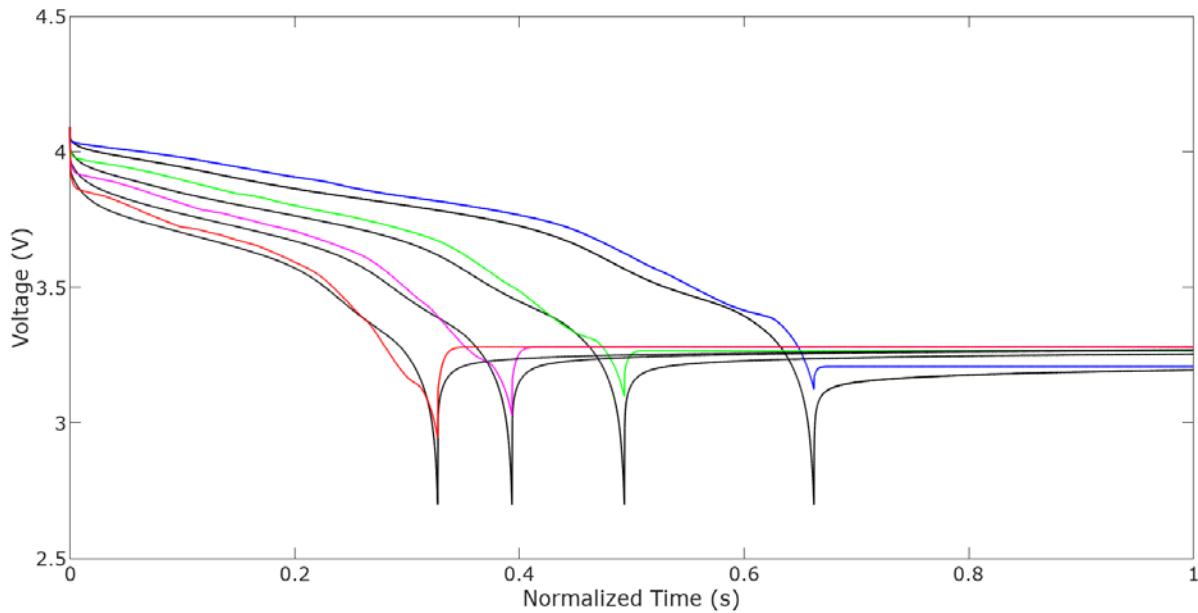

Figure 12: Comparison of the experimental (in black) and analytical voltage profiles for discharge pulses at C-rates of 1C (in blue), 2C (in green), 3C (magenta) and 4C (red) for a type E cell at 25°C

The figure 13 represents the SOC shift dynamism defined by the equation:

$$SOCshift = SOCshift_0 e^{-\frac{t-t_0}{\tau}} + SOCshift_{SS}(1 - e^{-\frac{t-t_0}{\tau}}) \qquad (16)$$

Where $SOCshift_0$ is the SOC shift at the previous change of the current, t_0 marks the previous current change and $SOCshift_{SS}$ is the final equilibrium SOC shift at the new current value. We chose $SOCshift_{SS}$ equal to f during the discharge period and equal to 0 once the current removed, and $SOCshift_0$ by opposition.
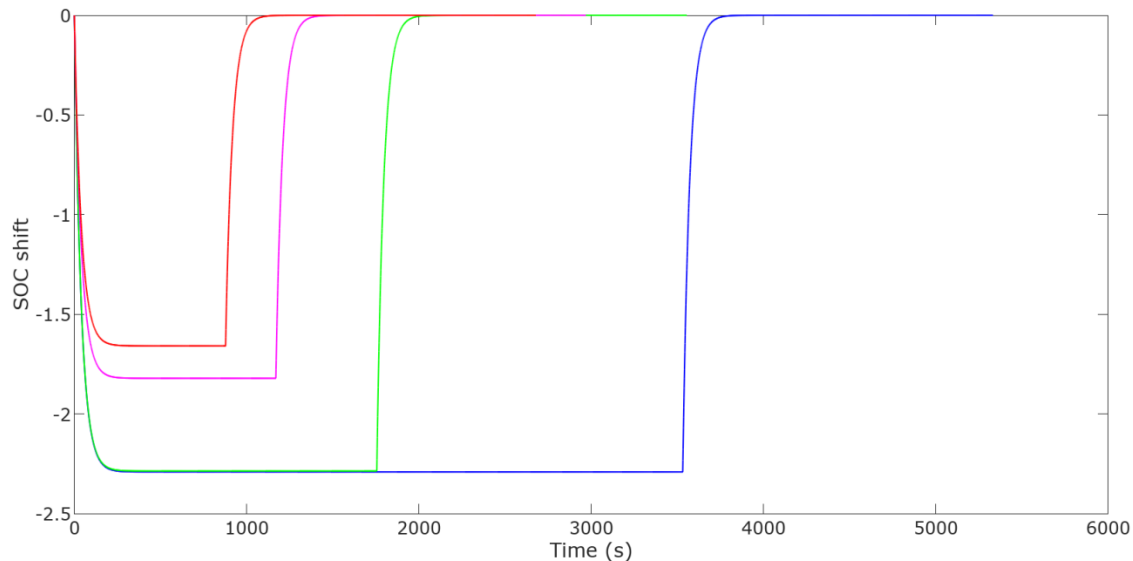

Figure 13: SOC shift dynamism for discharges at C-rates of 1C (in blue), 2C (in green), 3C (magenta) and 4C (red) for a type E cell at 25°C

5- Conclusion

The present paper had the ambition to guide LS-DYNA users in defining properly the input Randles battery parameters needed in battery simulation. It proposed one method judged quick and accurate by the practice but that should not be taken as an end. It has in particular been used to set up the input parameters of satisfactory battery abuse simulations presented in [2], paper also published this year in the context of the 15th International LS-DYNA Users Conference. The comparison method to a 0-D Randles model may also be used in the thermal parameters identification.

Appendix

Appendix A – Matlab Program Overview

A Matlab program has been used to test the parametrization process and is released to the users. It fits with the experimental data format from the team Ford and must therefore be adapted to fit with the users' ones. The following presents the structure of the code and gives the lines that need a particular attention from the users.

The program includes 7 .m files and 3 .txt data files.
The 7 .m files are: main.m, data_visualization.m, data_reading_by_user.m, data_reading_auto.m, getOCV.m, getComponents.m and getSOCshift.m. The 3 .txt data files are: C10test.txt, HPPCtest.txt and MultiRtest.txt.

- ➢ main.m
  - • loads the experimental data .txt files;
  - • gets the battery parameters Q and cQ;
  - • gets the values of the variables:
    - nbPulse: number of charge/discharges pulses of the HPPC test;
    - nbDischarge: number of discharge pulses of the multi C-rates test;
    - step – argument of getOCV: step between each SOC value in the SOCTOU definition;
    - plotOCV – argument of getOCV: boolean activating the plot of the curves representative of the OCV in function of the battery charge and of the SOC (see figure 7);
    - plotPulse, plotResultsComparison – arguments of getComponents: booleans activating the plot of the curves representative respectively of the experimental voltage profile for every pulse (see figure 8) and of the comparison experimental/analysis voltage for every pulse (see figure 9);
    - plotV_init, plotSOCshift, plotV_shifted – arguments of getSOCshift: booleans activating the plot of the curves representative respectively of the comparison experimental/analysis voltage dependent of the SOC for every discharge (see figure 12), of the dynamic terms SOCshift (see figure 13) and SOCshifted and of the comparison experimental/analysis voltage dependent of the SOCshifted for every discharge;
  - • calls the 5 functions data_visualization, data_reading_by_user or data_reading_auto, getOCV, getComponents and getSOCshift;
  - • extends manually the values of SOCTOU, R0_D, R0_C, R10_D, R10_C, C10_D and C10_C for extremes SOC;
  - • saves the data in .txt files.

- ➢ data_visualization.m
  plots the experimental results (see figures 3, 5 and 6).

- ➢ data_reading_by_user.m
  records the experimental notable points defined by the user.
  This points are: for the C/10 test the charge/discharge starting and ending points; for the HPPC test the charge/discharge starting and ending points of every pulses (see figure 8); for the multi C-rates test the discharge starting and ending points of every high discharges.

- ➢ data_reading_auto.m
  records automatically the experimental notable points from the .txt files.
  The function substitutes to the previous function data_reading_by_user. The users must however pay attention to the if-s conditioning the record of the points.

- ➢ getOCV.m
  calculates the value of the OCV in function of SOCs going from 0 to 100 with a step given by the variable step.
  The steps are described in part 4-1.

- ➢ getComponents.m
  is called for every pulse and, for every pulse, defines its profile, extracts the relaxation period, calculates the components value by a linear least squares algorithm, and proposes the comparison between the experimental voltage and the one calculated with the optimized components values.
  The steps are described in 4-2.
  The function must be re-called if the HPPC test is repeated for different battery cell operating temperatures.

- ➢ getSOCshift.m
  does a first comparison between the experimental voltage and the one calculated with the optimized components values, calculates the SOC shift parameters f and τ following the steps described in 4-3, calculates the SOC shift on the discharge period and on a larger period allowing to visualize completely the SOC shift dynamism given by the equation (16), deduced the SOC shifted and does a final comparison between the experimental voltage and the one calculated with the optimized and shifted components values.
  During the initialization, the end of the discharge is shifted by 1780 for plot purposes. This value depends uniquely of the associated experimental data and should be modified to take into account the user's data.
  The function must be modified to take into account additional discharges and with different battery cell operating temperatures.

The code is released under Matlab and Octave versions: please contact the Author to get a copy.

References

[1] Pierre L'Eplattenier, Iñaki Caldichoury, James Marcicki, Alexander Barlett, Xiao Guang Yang, Valentina Mejia, Min Zhu, Yijung Chen, *A Distributed Randle Circuit Model for Battery Abuse Simulations Using LS*-DYNA, 14th International LS-DYNA Users Conference
[2] Jie Deng, Min Zhu, Chulheung Bae, Theodore Miller, Pierre L'Eplattenier, Sarah Bateau-Meyer, *Safety Modeling of Lithium-ion Batteries under Mechanical Abuse*, 15th International LS-DYNA Users Conference