

COMPUTATIONAL MODEL OF A BATTERY AND SIMULATION OF CHARGE AND DISCHARGE PROCESSES

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ABSTRACT

The battery is an ever-present equipment in any electrical system even though the purpose of its application is different from one system to another. He serves as a main power supply for an electronic device or a secondary power source to avoid power shortage in uninterruptible power supply, or an energy storage for the renewable energy generator. Due to the non-uniqueness of its application, obtaining a flexible model of a battery is of interest in order to ease its integration with any system. The present work is devoted to this purpose. The modeling method is based on the combination of the electrochemical governing law and the Thevenin electrical model. An algorithm-based simulation is then developed. This in order to visualize the evolution of the open circuit voltage and the state of charge evolution during charge and discharge process of a battery. As the theory suggest, it is noticed that the open circuit voltage is linked with the remaining capacity. The future work is to model the rate of change of the capacity toward a given charging voltage waveform. This in order to optimize the charging process.

Keyword: - State of charge of a battery, electric charge transfer, open circuit voltage, energy conversion, equivalent model.

1. INTRODUCTION

From handheld electronic device to renewable electrical energy generator system, passing through the electric vehicle, the battery play an important role in various electrical system. As the battery involve a chemical reaction, the charging and discharging process need a closer attention. In fact, an overcharging or a deep discharge are both destructive and shorten the battery lifetime. The State of Charge (SoC) is the key parameter to survey for controlling these processes. The evolution of this parameter cannot be read directly with an existing measuring device. Various study and experimental result shows that it is linked intimately with the open circuit voltage. This relation combined with the current counting technique are exploited in the most of the actual battery management system.

The purpose of the present work is to derive a computational flexible model of a battery in order to ease its integration with a given system. This is achieved by considering the electrochemical governing law of a battery combined, the electrical equivalent model and a numerical computation.

Since system modeling is prediction oriented, the results from the technique used in battery management system are post process and exploited only to validate the result of the obtained model.

2. GENERAL CONSIDERATION

The battery is a result of an association of cells. A cell is made of two electrodes with a metallic connector for the external connection purpose. These electrodes are immersed inside electrolyte which allow the ion transfer between them. During discharge process, the positive electrode undergoes a reduction reaction (gain of electron) while an oxidation reaction (loss of electron) occurs at the negative electrode. The flow of the charged particle inside the battery cells determines the name assignation of an electrode.

However, for a secondary battery, the discharging process is considered by convention. The positive electrode is called Cathode since a negative current flow from this electrode to the other into the electrolyte. The negative electrode is called Anode.

Figure. 1 shows a two dimensional configuration of a cell from which our study is based.

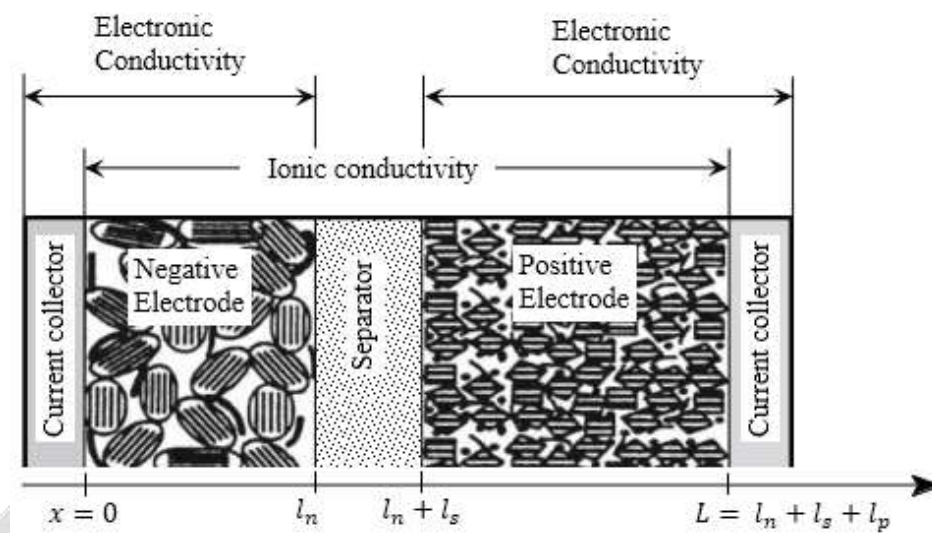


Fig -1: Two dimensional standard representation of a battery cell [1]

2.1 Relationship between capacity and active material quantity

Whenever a battery is charged or discharged, an electron flow in the external circuit occur. The electric current delivered by the cell to the external circuit is matched by the ionic current within the cell. For the discharge process, the negative electrode supply electron and the reaction is related by the following equation [2]:



Where each M^{x+} ion gives up n number of electrons in order to form the oxidized product. The equivalent number of moles of reactant consumed by the passage of a current i , flowing for a period $[0; \tau]$ is given by:

$$N_M = \frac{1}{nF} \int_0^\tau i(t) dt \quad (2)$$

Where $F = 96\,490 \text{ C.mol}^{-1}$ represent the Faraday's constant.

Conversely, if N_M represents the total number of moles of M^{x+} of the anode active material, available for reaction, the theoretical maximum capacity of the cell, which is the total amount of charge that could be supplied to the external circuit is given by:

$$Q_T = \int_0^{t_{fin}} i(t) dt = nFN_M \quad (3)$$

with t_{fin} the final time to reach the total capacity. Since a cell is composed with a negative and positive electrode, the reaction equation for the later electrode is given by:



An equivalent number of moles N_p at this side is being reduced. The maximum capacity is then given by the smaller of the two quantities nFN_M and $n'FN_p$. Recall that n (respectively n') represents the number of electrons given by the oxidized material (respectively received by the reduced material).

For operational reasons, most of the cell is positive or cathode-limited, which means $nN_M > n'N_p$.

2.2 Energy content of a cell

As a matter of fact, the battery is a device which convert chemical energy to electrical energy and vice versa. It is worthwhile to consider the energy content of a cell depending on its characteristics. Under a constant voltage, a current flow means that a work is done in the cell. For one mole of reaction, the expression of the maximal electrical work is:

$$W_{max} = nFV_{cell} \quad (5)$$

By definition:

$$W_{max} = -\Delta G \quad (6)$$

where ΔG is the Gibbs free energy change associated with one mole of reaction. It is the difference between the molar Gibbs free energy of products and reactants [3].

$$\Delta G = \Delta G_{products} - \Delta G_{reactants} \quad (7)$$

Hence the link between electrical energy and chemical energy is given by:

$$\Delta G = -nFV_{cell} \quad (8)$$

2.3 Open circuit voltage and capacity

As given from datasheets, the open circuit voltage for a fully charged battery is neatly greater than when it is fully discharged. Since in the ideal case, the battery voltage should be constant during its operation, it is noticed that the open circuit voltage is linked with the remaining capacity, called State of Charge (SoC).

As a battery cell include a positive and negative electrode, the expression of the open circuit voltage is given by:

$$V_{oc} = V_{eq+} - V_{eq-} \quad (9)$$

where V_{eq+} and V_{eq-} are respectively the potential of the positive and the negative electrode at equilibrium toward the Standard Hydrogen Electrode [4].

By considering the general half reaction at one electrode:



ν represents the stoichiometric coefficients. The cell reaction toward hydrogen is:



At a thermodynamic equilibrium where the temperature and the pressure are considered constant, the potential of an electrode is given by the Nernst equation [2]:

$$V_{eq} = V_0 - \frac{RT}{nF} \ln \left(\frac{a_R^{\nu_R} a_{H^+}^{\nu_{H^+}}}{a_O^{\nu_O} a_{H_2}^{\nu_{H_2}}} \right) \quad (12)$$

with V_0 the standard potential of an electrode toward the standard hydrogen electrode, and a_i the activity of species i . Since $a_{H^+} = a_{H_2} = 1$, Eq. 12 becomes:

$$V_{eq} = V_0 - \frac{RT}{nF} \ln \left(\frac{a_R^{\nu_R}}{a_O^{\nu_O}} \right) \quad (13)$$

a_R and a_O are respectively the activity of the reduced and oxidized species. The similar equation is valid for the other electrode so that Eq. 9 may be satisfied.

In a more general form, with $A, B, \dots$ the reactants and $P, Q, \dots$ the products, for an overall cell reaction as follow [2]:



The expression of the open circuit voltage is:

$$V_{oc} = V_0 - \frac{RT}{nF} \ln \left(\frac{a_P^{\nu_P} a_Q^{\nu_Q} \dots}{a_A^{\nu_A} a_B^{\nu_B} \dots} \right) \quad (15)$$

In fact, the deviation of a solution from its ideal behavior can be represented by the means of the activity coefficient such that:

$$a_i = \gamma_i \left(\frac{C_i}{C_0} \right) \quad (16)$$

where γ_i the dimensionless activity coefficient, C_i the concentration of the solute and C_0 a standard concentration. By assuming that the system is ideal, the activity coefficient can be approached by unity. Therefore, the open circuit voltage can be written also as a function of species concentration as follow:

$$V_{oc} = V_0 - \frac{RT}{nF} \ln \left(\frac{C_P^{\nu_P} C_Q^{\nu_Q} \dots}{C_A^{\nu_A} C_B^{\nu_B} \dots} \right) \quad (17)$$

This last expression relate the interdependence between the open circuit voltage and the products-reactants concentration.

Considering the discharge mechanism, the positive ion (cation) flow from the negative to the positive electrode while the negative ion (anion) flow in the opposite direction. Obviously, for a secondary battery, this process must be reversible so that the charging process can be achieved. This ion displacement lead to consider the variation of the active material quantity which define also the remaining capacity and then the State of Charge.

At the fully charged state:

$$SoC = 100 \%$$

the number of mole of the active material at the positive electrode side is N_P so that the initial concentration of this material is:

$$C_P(t=0) = \frac{N_P}{v_{ref}} \quad (18)$$

where v_{ref} a given reference volume. During Δt discharge time, let $N_{P_{extracted}}(\Delta t)$ the number of mole of the positive ion being extracted from the positive material and its concentration become:

$$C_P(t = \Delta t) = \frac{N_P - N_{P_{extracted}}(\Delta t)}{v_{ref}} \quad (19)$$

This ion subtraction from the positive electrode imply an ion supply to the negative electrode. The negative material concentration can be obtained by analogy as:

$$C_N(t = \Delta t) = \frac{N_N + N_{P_{extracted}}(\Delta t)}{v_{ref}} \quad (20)$$

These two last equations show that the concentration is linked with the active material quantity. By deduction, according to Eq. 15, the open circuit voltage of a battery cell depends on the remaining capacity, hence the State of Charge (SoC).

3. CELLS UNDER CURRENT FLOW

3.1 Electrical current and chemical reaction rate.

As stated above, a current flow through the load of the battery mean a charge (ion) transfer inside the battery. Introducing the derivative at both side of the Eq. 2 we have:

$$\frac{dN_M}{dt} = \frac{i}{nF} \quad (21)$$

This equation relate the rate of the material consumption during a current flow. Sometimes, it is convenient to introduce the current density by express this rate of current per unit area, the Eq .21 become:

$$\frac{1}{A} \frac{dN_M}{dt} = \frac{i}{AnF} = \frac{j}{nF} \quad (22)$$

where j is the current density expressed in $A.cm^{-2}$

3.2 Internal resistance and overvoltage.

Here we assume that cell and battery may be used indifferently because this latter is merely an association of two or more cells. A current flow, during charge or discharge process undergoes a certain resistance due to the physical and chemical properties of the cell. This resistance induce a voltage drop relatively to the open circuit voltage which can be noticed during discharge. Let V_L the applied voltage to a given load, due to the internal resistance, the expression of V_L is:

$$V_L = V_{oc} - Ir_b \quad (23)$$

Where r_b the internal resistance of the battery. This resistance can be divided in two main resistance according to its own cause:

- The ohmic resistance due to the electrical properties of each phase of the cell which are current collector, electrode, electrolyte and separator. Let r_{ohm} this ohmic resistance, thus we have:

$$r_{ohm} = \sum_j \frac{l_j}{\sigma_j A_j} \quad (24)$$

l_j the length, σ_j the electric conductance and A_j the area of each component.

- The resistance to species transfer which include the migration (movement of a charged body under the influence of an electric field), diffusion (movement of a species under the influence of a gradient of chemical potential) and convection (generally a fluid flow).

Recalling that a current flow means a species transfer, the flux of species $J_i(x)$ is governed by the Nernst-Plank equation [4]:

$$J_i(x) = -D_i \frac{\partial C_i(x)}{\partial x} - \frac{z_i F}{RT} D_i C_i \frac{\partial \phi(x)}{\partial x} + C_i v(x) \quad (25)$$

With D_i the diffusion coefficient, C_i the concentration, $\phi(x)$ the potential function and $v(x)$ the velocity with which a volume element in solution moves along axes. This equation show that the species transfer is subject to various physical phenomenon, thus undergo a resistance which imply an overall electric resistance also.

Let r_{st} the resistance associated with this species transfer. This latter can be split again in two main component which are the resistance to mass transfer r_{mt} , and the resistance to charge transfer r_{ct} . Their determination involve a further investigation of the above mentioned species flux equation. However, the total internal resistance r_b can be written as:

$$r_b = r_{ohm} + r_{st} \quad (26)$$

One method to approximate its value is the deduction from the polarization curve. This curve plot the load voltage V_L against the current capability of the cell.

A method commonly used to evaluate the internal resistance of a given electrical power generator is the open circuit test, to measure the open circuit voltage and the short circuit test to measure its maximum current capability. Similarly to this method, the plot of the load voltage V_L against the current I being delivered called polarization curve allow to measure the internal resistance of a battery. Figure. 2 shows a typical polarization curve [1] [2]. The voltage drop $\eta(I)$, lead to the measure of the internal resistance such that:

$$\eta(I) = V_{oc} - V \quad (27)$$

$$r_b = \frac{\eta(I)}{I} \quad (28)$$

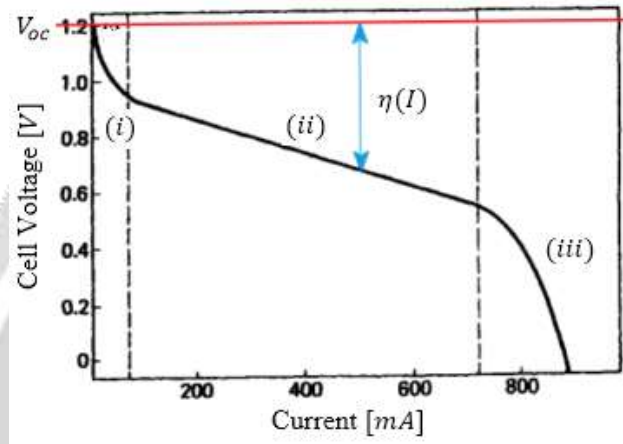


Fig -2 Typical polarization curve of a battery cell

In a general manner, the slope in the region (ii) gives the ohmic resistance:

$$r_{ohm} = \frac{dV}{dI} \quad (29)$$

3.3 Electrical model of a battery.

As the main purpose of a battery to deliver a continuous voltage, intuitively a Thevenin equivalent circuit may be used to approach its model with:

$$V_{Th} = V_{oc}$$

$$R_{Th} = r_b$$

Where V_{th} and R_{th} are respectively the Thevenin equivalent voltage source and resistance. However, V_{oc} decrease slightly with the State of Charge. The physics of the species transfer (mass and/or charge) induce a capacitor effect in addition to r_{st} . Let C_{st} this capacitor, the Fig. 3 show the electrical model of a battery derived from the Thevenin model with C_{st} in consideration and the load resistance R_L connected.

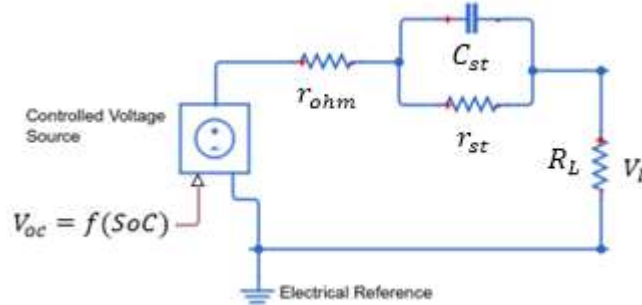


Fig -3 Electrical model of a battery

Here, V_{oc} is a controlled voltage source since its value is linked with the State of Charge. In order to obtain the load voltage V_L , we apply the Kirchoff Voltage Law.

$$V_L = R_L i \quad (30)$$

$$V_L = V_{oc} - r_{ohm} i - V_{st} \quad (31)$$

i is the total current in the circuit, let i_1 the current passing through r_{st} and i_2 through C_{st} , we have:

$$i = i_1 + i_2 \quad (32)$$

With:

$$i_1 = \frac{V_{st}}{R_{st}} \quad (33)$$

and

$$i_2 = C_{st} \frac{dV_{st}}{dt} \quad (34)$$

We have:

$$\begin{aligned} R_L \left(\frac{V_{st}}{R_{st}} + C_{st} \frac{dV_{st}}{dt} \right) &= V_{oc} - r_{ohm} \left(\frac{V_{st}}{R_{st}} + C_{st} \frac{dV_{st}}{dt} \right) - V_{st} \\ \left(\frac{R_L + r_{ohm}}{r_{st}} + 1 \right) V_{st} + (R_L + r_{ohm}) C_{st} \frac{dV_{st}}{dt} &= V_{oc} \end{aligned} \quad (35)$$

Assuming that $V_{st}(0) = 0$, in solving this differential equation, we have the expression of V_{st} :

$$V_{st}(t) = \frac{r_{st} V_{oc}}{R_L + r_{ohm} + R_{st}} + \left(V_{st}(0) - \frac{r_{st} V_{oc}}{R_L + r_{ohm} + R_{st}} \right) \exp \left(\frac{-(R_L + r_{ohm} + r_{st})t}{r_{st}(R_L + r_{ohm})C_{st}} \right) \quad (36)$$

From Eq. 32, 33, 34 we can derive the expression of $i(t)$ such that:

$$i(t) = \frac{1}{r_{st}} V_{st}(t) + C_{st} \frac{d}{dt} V_{st}(t) \quad (37)$$

and thus $V_L(t) = R_L i(t)$

4. SIMULATION

The simulation allow us to observe the evolution of the electrical value, the load voltage during the discharge and the open circuit voltage during charge. The successive values are obtained programmatically where the discharge and charge are treated separately.

As we have already mentioned, the variation of the open circuit voltage is intimately linked with the remaining capacity. This variation must be taken into account in the model. It can be estimated and established from the very construction in factory according to the Eq. 17. However, in most case, it is not given by the constructor or the vendor. Another way to provide it is to perform a curve fitting from experimental data.

In this present work, we used the model derived from the Nernst equation given by [5]:

$$V_{oc} = V_0 - \frac{RT}{nF} \ln \left(\frac{x}{1-x} \right) \quad (38)$$

where x is the normalized consumed capacity, let C_N the nominal capacity. From the Eq. 3, for the discharge process, the remaining capacity C_N can be obtained by:

$$C_r = C_N - \int_0^t i(t) dt$$

Thus

$$x = \frac{C_N - C_r}{C_N} \quad (39)$$

And for the charging process, we replace x in Eq. 38 by $1 - x$.

The simulation is done for the calculation to be flexible. The charge and discharge process are treated separately.

4.1 Overview of the algorithm on discharge and charge process

Here, our main concern is the evolution of the voltage V_L (respectively V_{oc}) on discharge (respectively on charge). The diagram in the Fig. 4 below shows an overview of the step in the Algorithm.

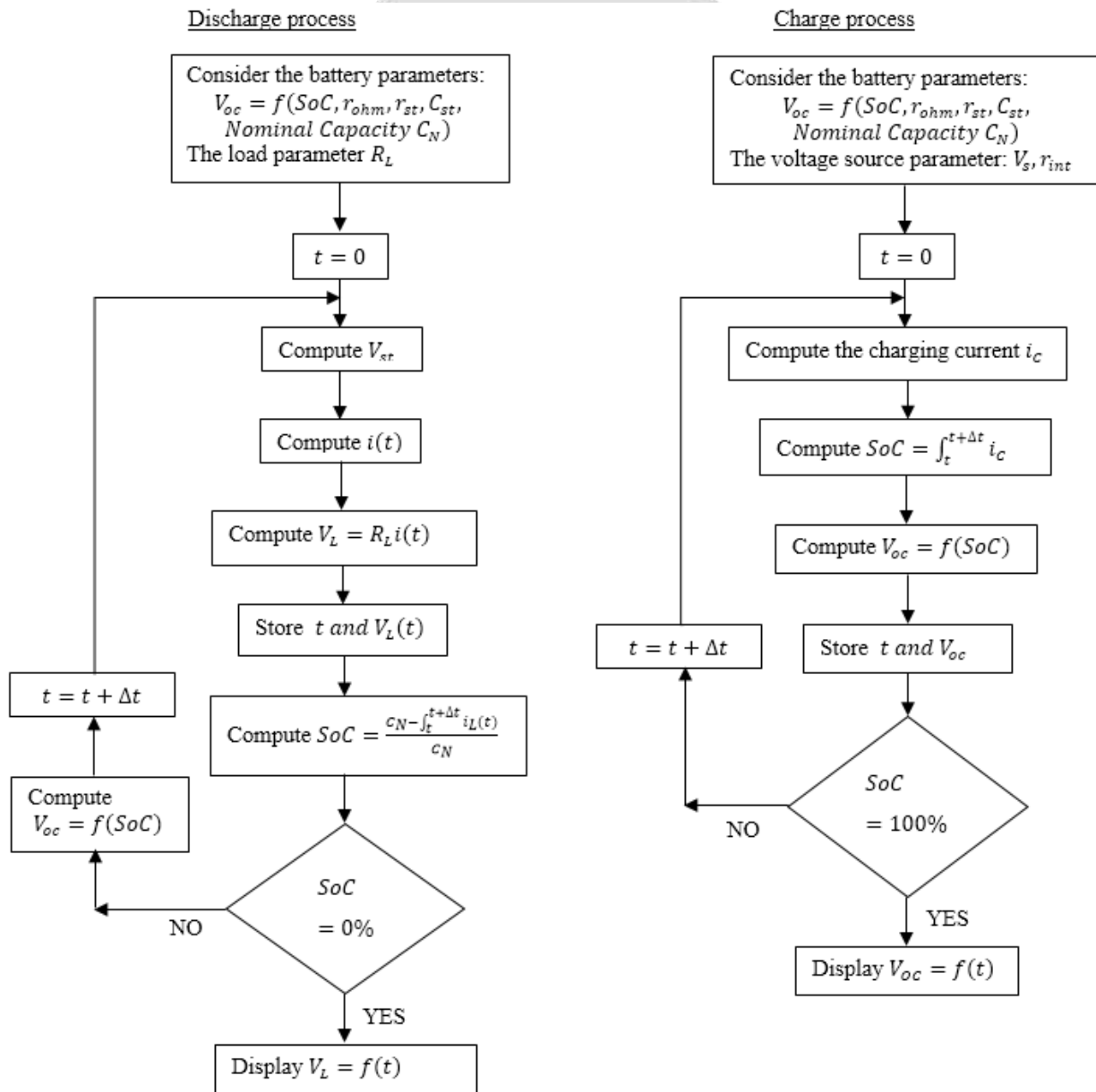


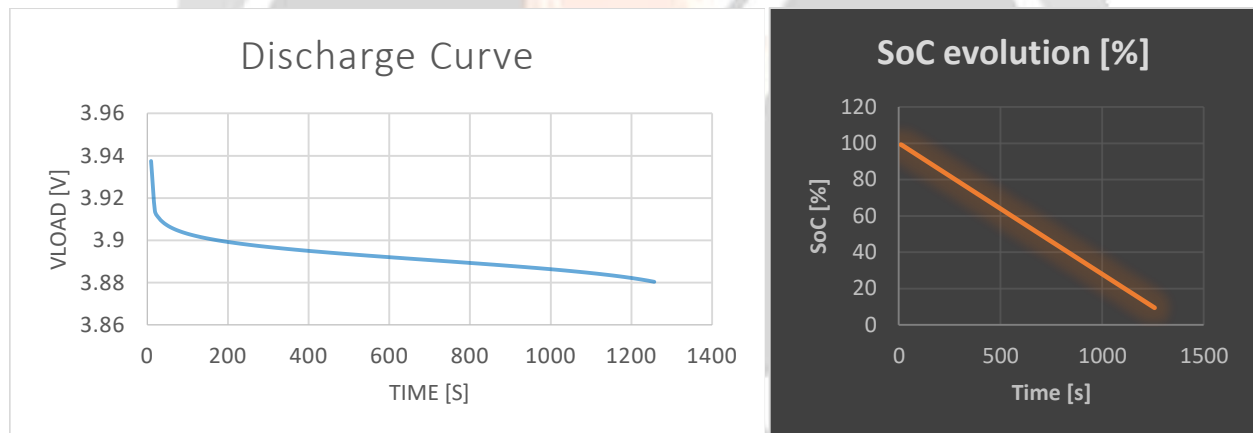
Fig -4 Algorithm for discharge and charge simulation**4.2 Simulation of the model.**

Figure. 5 shows the user interface for the discharge process while Fig.6 a) and b) the results for two different R_L .

The 'Discharge Simulation' window contains the following parameters and controls:

Parameter	Value
Rload [ohm]	3
Rohm [ohm]	0,04
Rct [ohm]	0,06
Cct [Farad]	0,000001
Voc init [V]	4,2
Capacity [Ah]	1

Buttons: RUN, REDUCE, EXIT

Fig -5 User interface for the discharge process**Fig -6 a)** $R_L = 1,5 \Omega$

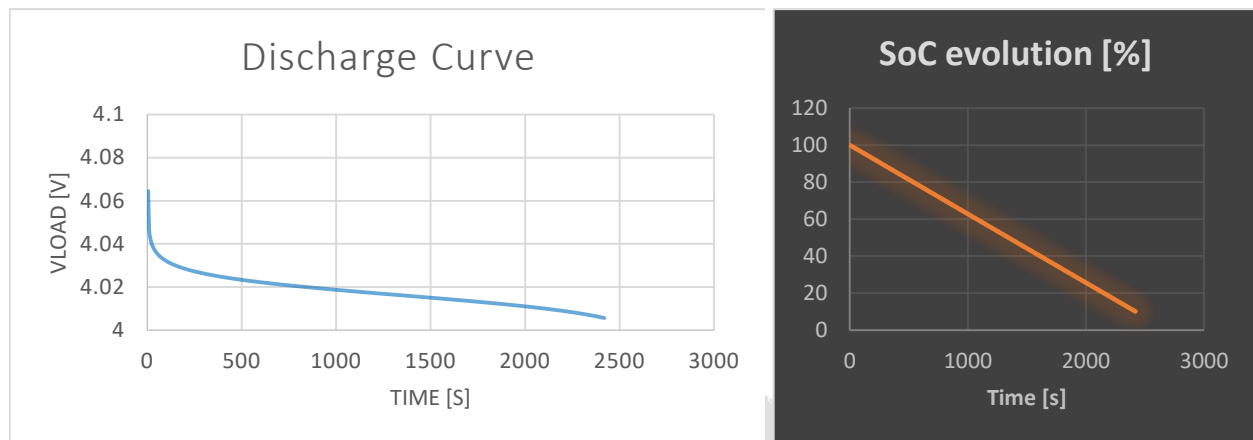


Fig -6 b) $R_L = 3 \Omega$

Fig -6 Discharge curve for a) $R_L = 1,5 \Omega$, b) $R_L = 3 \Omega$

Figure. 7 shows the user interface for the charge process while Fig.8 a) and b) the results for two different nominal Capacity 1 Ah and 2,5 Ah

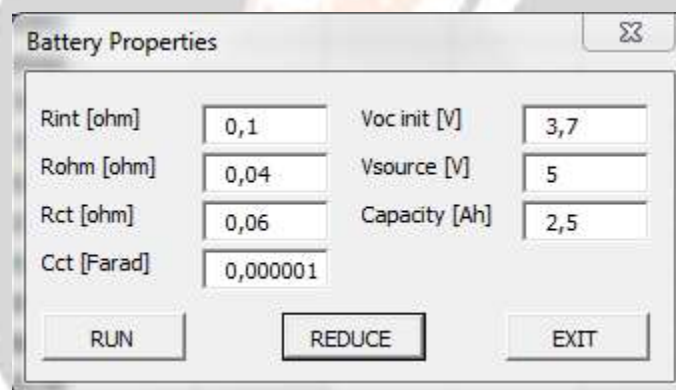


Fig -7 User interface for the charge process

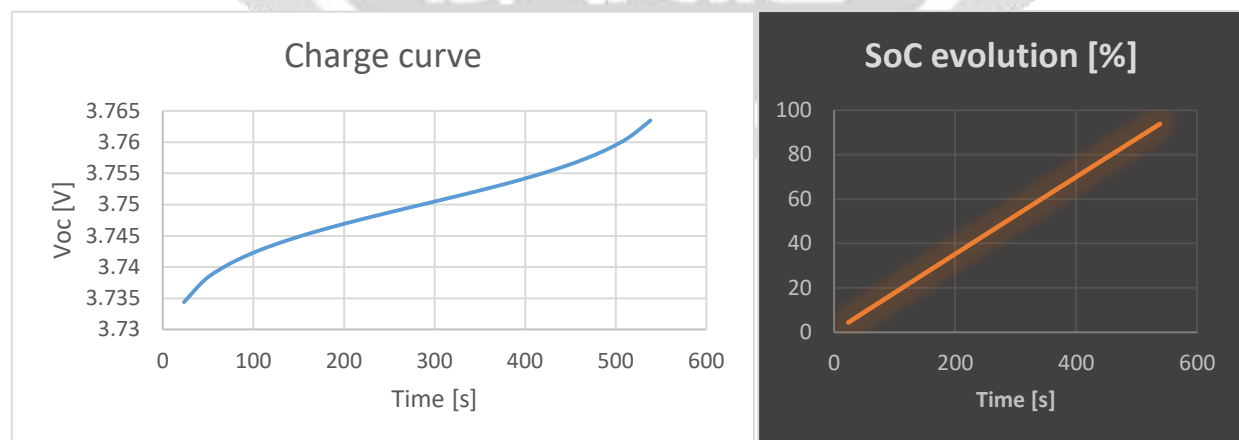


Fig-8 a) $C_N = 1 \text{ Ah}$

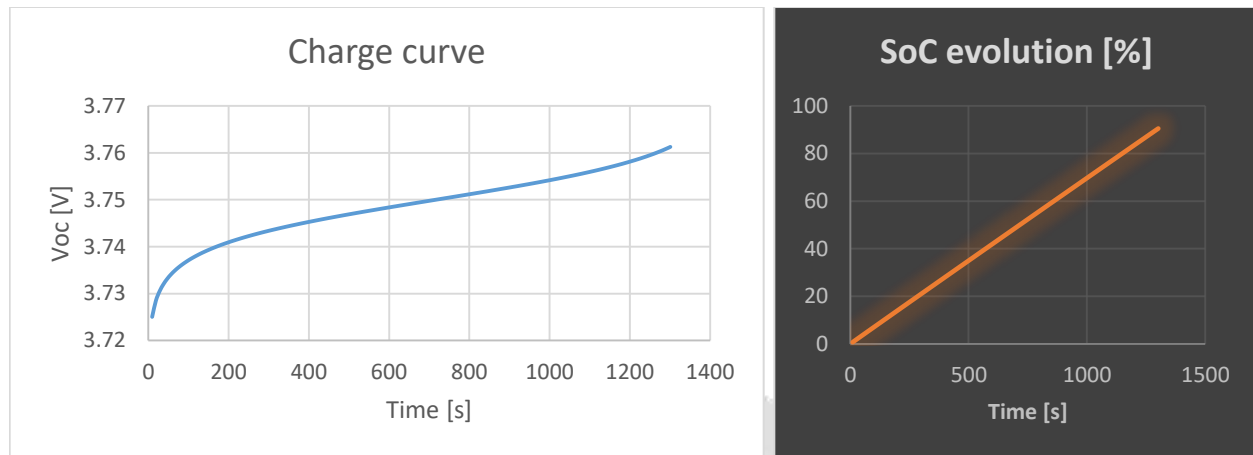


Fig-8 b) $C_N = 2,5$ [Ah]

Fig -8 Charge curve for a) $C_N = 1$ Ah, b) $C_N = 2,5$ Ah

The computation is performed with Excel and VBA programming. The needed parameter must be provided first via the user interface before running the simulation. The battery considered here is of a Lithium-ion type where the typical open circuit voltage at $SoC = 100\%$ is $4,2\text{ V}$ and $3,7\text{ V}$ at $SoC = 0\%$. The other parameters are: $r_{ohm} = 0,04\ \Omega$, $r_{ct} = 0,06\ \Omega$, $C_{ct} = 1\ \mu\text{F}$. These parameters can be modified as the battery type, or the capacity or the internal parameter change. For the charge process, we considered the internal resistance of the voltage source and the initial value of the open circuit voltage when the battery is fully discharged.

4.3 Discussion of the result.

In these simulation, the evolution of the load voltage is of interest for the discharge and the open circuit voltage for the charge.

For the discharge process:

- It can be observed that as the value of the load resistance increase, the duration for the battery to be fully discharged increase. This is because the current drawn from the battery decrease.
- The voltage drop from the starting value can be noticed also due to the internal resistance of the battery.

For the charge process:

- As the nominal capacity increase, the time it take to be fully charged is extended also for a constant voltage source.

For the two process:

- It can be noticed that the charge or discharge curve keep pace with $V_{oc} = f(SoC)$ curve. The accuracy of this last expression play an important role in the battery modeling. The closer to the real situation is the link between V_{oc} and SoC , the more reliable is the result. As we have already seen, V_{oc} depend strongly on the species concentration in each phase of the cell component. It is desirable if the data is furnished from the factory.
- The internal parameter such as r_{ohm} , r_{ct} and C_{ct} are also to be considered because they induce a deviation from the behavior of an ideal continuous voltage source.

Due to its flexibility, the model can be expanded and adapted to another system which involve an energy storage such as a hydroelectric generator.

5. CONCLUSION

The operational mode of the battery as an energy storage is the invertible conversion between electrical and chemical energy. The present work show the relation between these two different but bound processes within a battery. It has been shown that depending on the expression of the open circuit voltage as a function of the state of charge, the deliverable instantaneous power is not perfectly constant as the energy is being exhausted. The charging time also depend on rate of charge transfer, hence on the cells physical and electrical characteristics.

For the future work, a relation between the charging voltage waveform and the state of charge evolution is to be considered in order to improve the charging efficiency.

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