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Review on Lithium-Ion battery modeling for different applications

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ABSTRACT

Battery modeling is one of the most important functions in a battery management system for different applications such as electrical vehicles, This article focuses on state of the art of lithium-ion battery modeling by exploring different existing modeling methods, such as Electrochemical models, Analytical models and the equivalent electrical circuit. First, the characteristics of the lithium-ion battery for different applications are reviewed ,we chose to study this type of battery because it offers satisfactory characteristics compared to other battery types, then the different modeling methods have been explored, finaly a conclusion with suggestion of other modeling type such as fractional order model have been proposed to improve efficiency and precision of battery management system.

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1. INTRODUCTION

Today, there are many applications for energy storage systems. The batteries are the most famous. They are used in several industries, such as electric and hybrid vehicles, renewable energy systems and marine energy systems. Batteries are used as back-up in wind or photovoltaic energy conversion systems. They are implemented to store excess energy captured by wind power or sunlight using wind turbines in windy or sunny weather, as well as to release stored energy during stationary periods or during the night. In electric or hybrid trains and vehicles, a battery is used to store energy from the regenerative braking system and to return energy to the system when the train is in traction mode. They can increase the reliability of hybrid systems.

Different chemical batteries are widely used in these applications as: lead-acid, nickel cadmium (NiCd), nickel-metal hydride (NiMH) and lithium ion (Li-ion), Compared with other battery systems, Li-Ion battery offers many advantages such as lightness, high energy density and ease of manufacture, they also have excellent energy density, do not have memory effect and have a long lifespan. [1-6] The electrochemical behavior of the accumulator is at the origin of the two main sources of heat to which it is subjected. The Joule effect, called irreversible, results from the electrical nature of the battery, while the reversible heat comes from chemical reactions at the level of the electrodes. Optimizing a Li-Ion battery model for a given application necessarily involves saving a large amount of time and experimental effort, thus saving considerable time and money as well as having a good battery.

Precise modeling and simulation of this type of battery is necessary in order to examine its performance and different modeling approaches exist: electrical modeling, "black box" modeling, energy modeling, physicochemical modeling.

Modeling of electrical circuits is a useful model presented by many researchers. In the modeling of the electrical circuit, the electrical characteristics of the battery are taken into account and passive linear elements are used. Such models are presented in different papers [7-12].

"Black box" modeling connects the possible system responses to a specific type of stimuli, regardless of the mechanisms responsible for its behavior. The accumulator is represented by a black box with inputs and outputs that consist of physical quantities related to the operation and conditions of use. In general, inputs are composed of current, state of charge, temperature, and state of aging when it is possible to estimate it. The magnitude that we want to estimate at the output is generally the tension. The box consists of an estimator that is able to predict the values of the outputs according to the inputs. Examples of estimators are presented in [13-15].

Energy modeling models all energy flows within the electrochemical battery without the use of partial differential equations. It consists of processing energy flows of different types: electrical, thermal, or fluidic.

Physicochemical modeling is seldom used in the domain of electrical engineering. It uses the principles of chemistry and physics to describe the precise behavior of the battery cell. Its main interest is that it facilitates the understanding of the phenomena that limit the performance of the cells, and the fundamental mechanisms of the generation of the power, making it possible to further improve the batteries’ construction processes and design. These models require accurate and functional knowledge of many parameters (electrolyte concentration, diffusion coefficient, transfer coefficient, and electrode geometry). In [16-17], the authors present some electrochemical models for lithium-ion batteries.

In this paper, we present different types of modeling suitable for estimating the condition of a lithium-ion battery in the context of its use in battery management systems for different applications such as electric vehicles. These are electronic devices that include, among other things, computers on which we want to implement the observer. Their computing power and memory are very limited, which is why the model used must be numerically efficient and sober. After a general introduction in the first part. In the second part, we do a bibliographical review of electrochemical accumulators such as lithium-ion batteries available in the literature. In the third part, we present the different types of lithium-ion battery modeling, namely electrochemical models (such as Particle models (PM) and Porous electrode Model), then analytical models (such as Kinetic battery model) and finally models based on equivalent electrical circuits (such as First order model and multiple order model). And the last part is devoted to a conclusion that sums up all the work done in this article.

2. ELECTROCHEMICAL ACCUMULATOR

An electrochemical generator is a source of electrical energy obtained through the direct transformation of chemical energy. Three main categories of electrochemical generators exist, namely: batteries, accumulators and fuel cells. The history of electrochemical generators begins in 1800 with Alessandro Volta, who invented the non-rechargeable primary cell. This stack is formed by a stack of alternating copper and zinc disks. In alternations, there are separating washers soaked in brine (H2O + NaCl) which allow the conduction of the current. This process makes it possible to obtain a generator formed of a zinc anode and a copper cathode, the whole being bathed in an electrolyte (brine) thus ensuring the movement of the electrons. However, Volta's battery is not rechargeable. The photo of a voltaic pile can be found in Figure 1.

Later in 1859, Gaston Planté, discovering the reversibility of electrical chemical reactions thanks to the reversal of the direction of the current, invented the lead accumulator. It is composed of lead alloy grids pasted with a mixture of sulfuric acid, lead oxide and water which constitutes the active ingredient. In 1899, this technology enabled an electric car in the shape of a torpedo to travel 100 km / h [18]. It was the first type of rechargeable battery marketed. Lead-acid batteries are still used in vehicles today for 12V and 15V power supplies. The success of this type of battery is due to the low cost of lead and sulfuric acid, their ease of manufacture and their lifespan of a few years [19]. The photo of a lead accumulator can be found in Figure 1.

Nickel-Cadmium (Ni - Cd) batteries have replaced lead batteries because they are more robust and powerful. In 1899, these accumulators were used for the electric vehicle "Jungner" and in 1900 for "Edison". However, the high cost and the very high toxicity limit the use of this type of accumulator [19].

Marketed in 1990, Nickel-Metal-Hydride (Ni –MH) batteries make it possible to overcome the toxicity of cadmium and have energy densities 30% higher than those of Ni-Cd batteries. In addition, these batteries operate at low temperature and have a low manufacturing cost. However, the use of these batteries has been reduced since the advent of accumulators based on lithium. Indeed, Ni –MH batteries have very moderate specific energy densities, which do not meet the criteria for reducing the weight of accumulators imposed by on-board applications.

(a) The Voltaic battery (b) Gaston Planté's battery.
Figure 1. Electrochemical generators

In 1991, the first rechargeable batteries based on lithium were marketed by the Japanese manufacturer Sony [20]. This technology quickly becomes predominant because of its performance in terms of specific energy, load capacity and electromotive force (emf). Table 1 summarizes these various battery technologies with their characteristics.

Table 1. Comparative table of the various battery technologies.

Type	EMF	Number of cycles	Charging Efficiency (%)	Massic Energy (Wh/kg)	volume energy density (Wh/l)	T (°C)
lead-acid	2, 1	500 to 1200	−	15 to 45	40 − 80	−40 to 40
Nickel-Cadmium	1, 2	≈ 2000	60	30 to 60	80	−20 to 60
nickel metal hydride	1, 2	500 to 1200	60	100	200	−20 to 60
Lithium-Polymer	3, 7	≈ 1000	−	100 to 130	140 − 435	−40 to 40
Lithium-ion	3, 6	1000 to 10000	95	150	300	−20 to 60

2.1. The lithium battery

The lithium battery is very attractive due to its high specific energy and energy density. This accumulator has the highest Electromotive force (EMF) as can be seen in Table 1. In addition, lithium is the lightest metal, making it possible to use high energy applications such as in electric vehicles. However, lithium batteries present risks of explosion or thermal runaway due to violent reactions between lithium metal and air [20]. These accumulators require close monitoring in order to ensure the safety of users. Nowadays, this function is fulfilled by the battery management system (BMS).

2.2. The Li-ion cell

The Li-ion battery is based on the reversible exchange of Li+ ion between the anode and the cathode. The anode and the cathode are separated by a material that allows lithium ions to pass through but not electrons: the separator. The separator can be a polymer film (polyethylene, polypropylene) or a microporous ceramic [19].

Nowadays, the anode is graphite and the cathode is often formed from lithiated transition metal oxide such as cobalt dioxide (CoO_2) or manganese (MnO_2). The electrolyte is often non-aqueous: a lithium salt in an organic solvent [21]. Figure 2 illustrates the operation of a Li-ion cell in discharge. The e^- electrons travel from the anode to the cathode through the outer circuit. The presence of negative charges (electrons) in the cathode attracts Li^+ ions which pass from the anode to the cathode through the separator to collect the missing charges. When all of the cycling lithium passes through the cathode, the battery is discharged. The reverse phenomenon occurs during charging and allows lithium to return to the anode. Equations 1 (respectively 2) represent the electrochemical reactions taking place in the cathode (respectively anode) when using the Li-Ion cell. The variable "M" represents the metal used at the cathode.

At the positive electrode (cathode) we have:

$$Li_{y-z}MO_2 + zLi^+ + z\,e^- \leftrightarrows LiyMO_2 \qquad (1)$$

At the negative electrode (anode) we have:

$$Li_xC_6 \leftrightarrows Li_{x-z}C_6 + zLi^+ + z\,e^- \qquad (2)$$

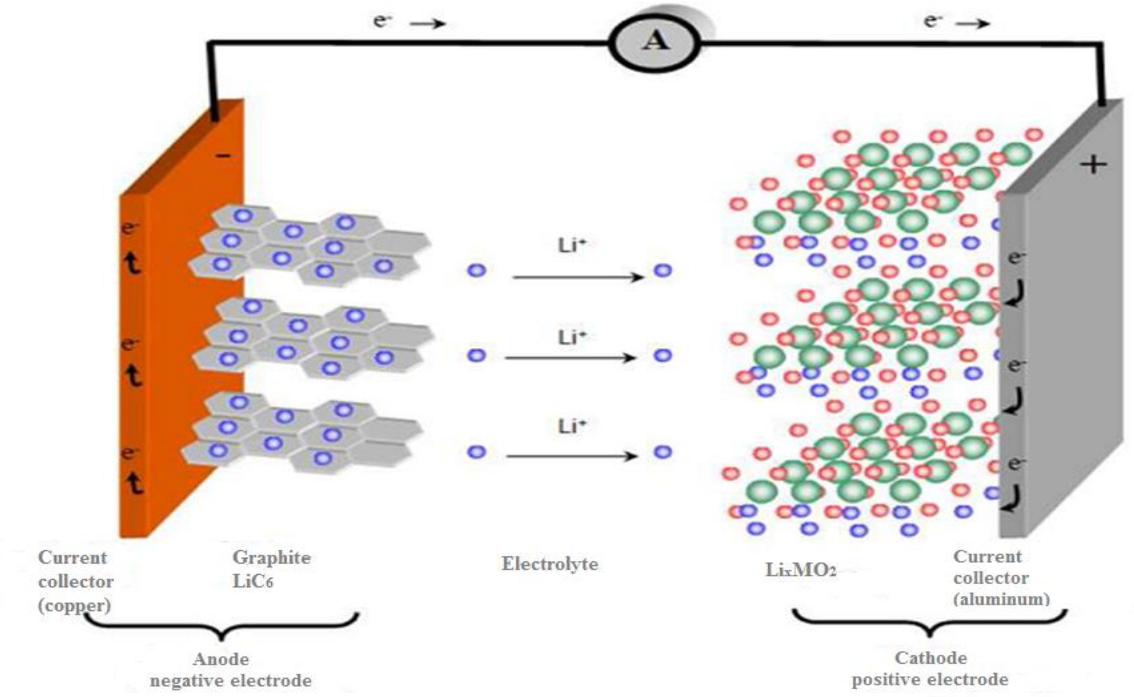

Figure 2. Structure of a Li-ion battery during a discharge

Lithium-ion batteries have attracted attention compared with other types of batteries since they have several advantages, high power density, high energy density, strong environmental adaptability, 'long life, and high cell voltage. However, there are several types of lithium-ion batteries, each type has its own advantages, such as LMOq which has a high specific power, LCO, which has a high specific energy, lithium-ion batteries NCA and NMC, which are the most thermally stable and cheapest, LTO, which has fast charging, long life and but higher cost and low specific energy [22]. Table 2 shows commercial lithium-ion batteries and their different characteristics.

Table 2. Comparison between commercial batteries of lithium-ion [23].

Abbrev.	LCO	LNO	LMO	NMC	LFP	NCA	LTO
Battery Name	Lithium cobalt oxide	Lithium nickel oxide	Lithium manganese oxide	Lithium nickel manganese	Lithium iron phosphate	Lithium nickel cobalt aluminum oxide	Lithium titanate
Year	since 1991	since 1996	since 1996	since 2008	since 1993	since 1999	since 2008
Nominal Tension (V)	3.7~3.9	3.6~3.7	3.7~4.0	3.8~4.0	3.2~3.3	3.6~3.65	2.3~2.5
Specific Energy (Wh/kg)	150~200	150~200	100~150	150~220	90~130	200~260	70~85
Charge (C)	0.7~1	0.7~1	0.7~1	0.7~1	1	0.7	1
Discharge (C)	1	1	1	1	1	1	10
Lifespan	500~1000	>300	300~700	1000~2000	1000~2000	500	3000~7000
Thermal Runaway (C)	150	150	250	210	270	150	-

3. LITHIUM BATTERY MODELING

3.1. Electrochemical models

Electrochemical models are the most sophisticated and rely on the kinetics of chemical reactions and transport equations [24]. They can to simulate the characteristics and reactions of a cell even before it is manufactured. The Pseudo-two-dimensional (P2D) model and the single particle model are among the most popular in this category [25]. According to paper [25], a battery management system (BMS) which would be based on an electrochemical model would have significant advantages over those based on empirical models.

Particle models (PM) : The electrochemical particle model is based on two principles. First, each electrode is modeled as a spherical particle within which the intercalation and deintercalation processes occur. In this model, variations in the potential or concentration of the electrolyte are ignored. The single particle model (SPM), Figure 3.a) has a much faster response than the porous electrode model (PEM), but fails to represent high current discharges [25]. The Multiple Particle Model (MPM), Fig. 3.b) has been proposed to take into account the size and varying conduction resistance of cathode oxide particles, mainly for LiFePo4 batteries [26-28].

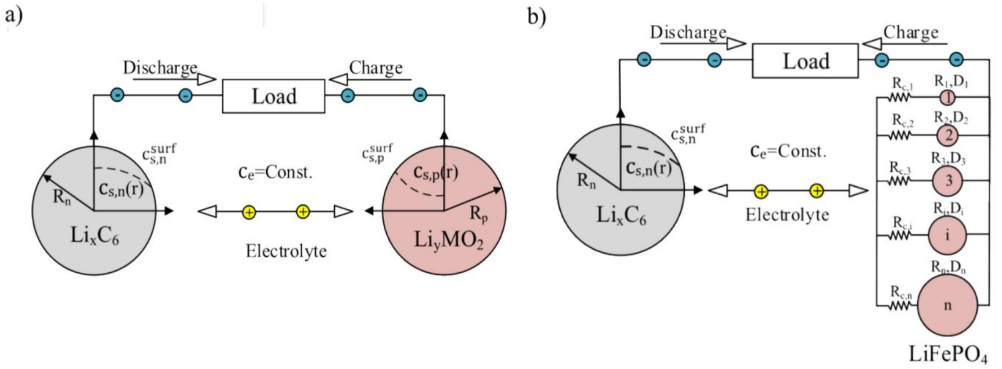

Figure 3 - Particle model: a) single, b) multiple [25]

Porous electrode Model : The PEM (Figure 4), is an evolution of the SPM taking into account the variation of the potential and the concentration. The PEM is based on kinetic equations, solution concentration theories and porous electrode theory [25, 29, 30]. This model is mainly used to study the local current density inside lithium-ion cells [31] with results close to experimental [32]. It captures the dynamics of lithium diffusion and the kinetics of charge transfer. It is a rigorous and precise model, but far too heavy for the computational capacities of an on-board system [33].

The physical models can be theoretical, analytical or electrochemical. In-depth knowledge of the materials and internal properties of cell construction, rarely provided by battery manufacturers, is required in the construction of these models. They are complex and difficult to implement.

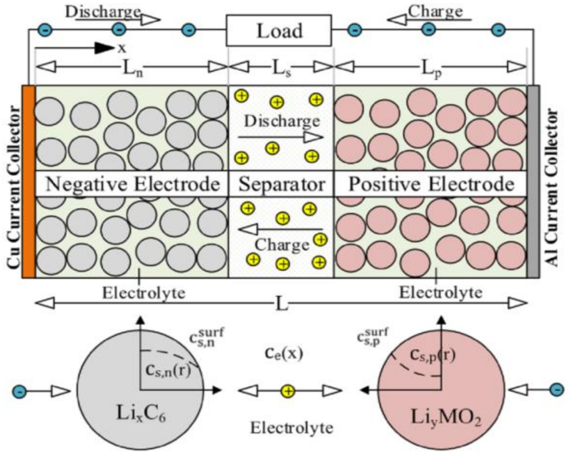

Figure 4. Porous electrode Model (PEM) [25]

3.2. Analytical models

The representation of the nonlinear kinetics of batteries by differential equation was the subject of research in the early of 1990s by Manwell and McGowan [34-35]. This model is better known as the Kinetec Battery Model (KiBaM). It is called kinetics because it uses the principles of the kinetics of chemical reactions as a basis. In this model based on a hydraulic analogy, the loads are distributed in two reservoirs: the reservoir of available loads y1 and that of limited loads y2 (fig.5). The current delivered i (t) by the battery corresponds to the liquid flow rate at the outlet.

Rakhmatov and Vrudhula [36] have developed a model based on the diffusion of lithium ions in the electrolyte which predicts the autonomy of a battery. Jongerden and Haverkot [37] denote similarities between the scattering model and the kinetic model, proving that the former was in fact the continuous representation of the latter. Analytical models cannot estimate voltage drop, aging, or heat generation. This makes this type of model unsuitable for use for any reason other than estimating the capacity of a battery. However, the hydraulic analogy is an interesting representation for understanding concepts and teaching battery science.

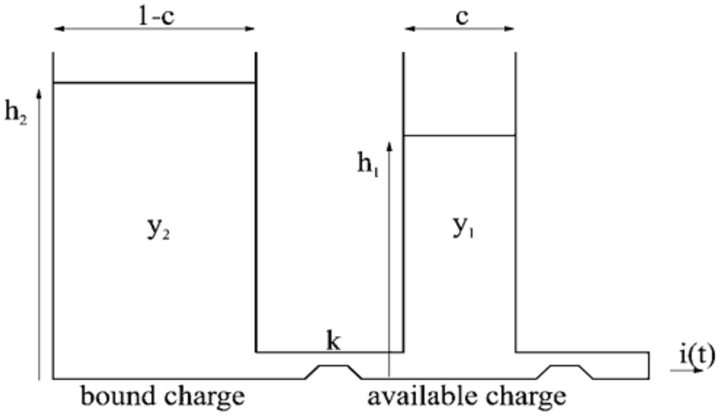

Figure 5. Kinetic battery model (KiBaM) [37]

3.3. The equivalent electrical circuit

The idea here is to represent the accumulator using an electrical circuit which takes its physical parameters into account. The classic approach to representing a voltage source is by an electromotive force in series with an ohmic resistance: U = E - RI. This simple approach makes it possible to quickly obtain an approximation of the behavior of the cell. You can add one or more R // C circuits depending on the precision you want to achieve.

First order model: This is a simple model which highlights the ohmic resistance (R0) of the cell as well as the phenomenon of diffusion (RD, CD). The variable Vt represents the terminal voltage of the cell, VD the voltage across the resistor RD in parallel with the capacitor CD, and OCV represents the no-load voltage of the cell.

$$\begin{cases} \frac{dV_D}{dt} = \frac{-V_D}{R_D C_D} + \frac{I}{C_D} \\ V_t = OCV - IR_0 - V_D \end{cases} \tag{3}$$

Multiple order model: This is the generalization of the first order model to a number n ≥ 2 of R // C circuits as illustrated in figure 6 and equation 4 for 1 ≤ i ≤ n. This approach increases the accuracy of the state of charge estimate because the low frequency behavior of the battery is better represented. But, this comes at the cost of greater model complexity.

$$\begin{cases} \frac{dV_{Di}}{dt} = \frac{-V_{Di}}{R_{Di} C_{Di}} + \frac{I}{C_{Di}} \\ V_t = OCV - IR_0 - \sum_{i=1}^{n} V_{Di} \end{cases} \tag{4}$$

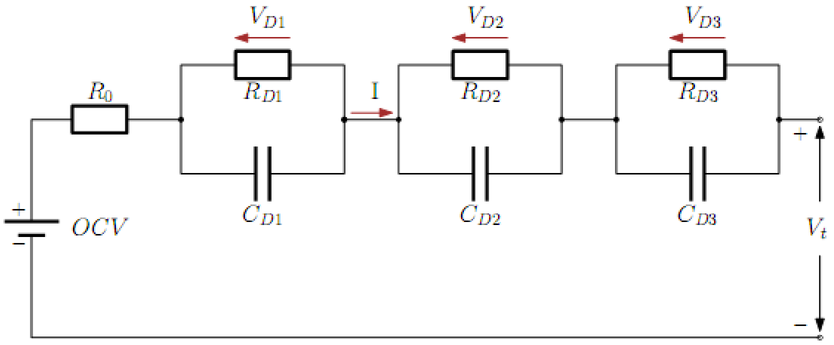

Figure 6. EEC model: Equivalent electrical circuit of order 3 [38].
OCV is the no-load voltage at rest (relaxed state) of the battery.

Consideration of hysteresis: Apart from the scattering which can to a certain extent be modeled by R // C branches, the Li-ion cell exhibits another non-linear behavior which is hysteresis. Indeed, when we observe the curve (f (SoC) = OCV) of the no-load voltage as a function of the state of charge of a Li-ion cell, we notice that the curves in charge and in discharge are different. This behavior of the Li-ion cell corresponds to a hysteresis phenomenon. Although very weak, this phenomenon still exists. Often in the literature, an average of the two curves is used to obtain a single representation of the relation f (SoC) = OCV. Sometimes, for more precision we find models allowing to better model this phenomenon. A distinction is made between the 0-state hysteresis model and the 1-state hysteresis model.

0-state hysteresis model: This is the simplest model, adding a term to the voltage measurement equation [39]. This term takes into account the fact that the hysteresis does not change sign directly with current. The system takes a long time to switch from one major hysteresis loop to another. The state equation of the system is given by:

$$\begin{cases} \mathrm{SoC}_{k+1} = \mathrm{SoC}_k - \left(\frac{n_i T_e}{600 Q_n}\right) I_k \\ V_t = \mathrm{OCV} - I_k R_0 - s_k M_0(\mathrm{SoC}_k) \end{cases} \quad (5)$$

where Te is the sampling period, SoC_k is the state of charge at instant k × Te, sk the sign of the current flowing through the cell and M_0 (SoC_k) is half of the difference between the curves f (SoC) = OCV charging and discharging depending on the state of charge SoCk and Qn the charging capacity of the cell in Ah.

4. CONCLUSION

In this paper, our aim was to explore the different modeling types of lithium-ion battery, we focused on lithium-ion battery due to its many advantages such as lightness, high energy density and ease of manufacture.

The literature offers a wide variety of lithium-ion battery models. It is often presented as being made up of three families. The first family is formed by physical models which describe batteries as electrochemical objects, since the main phenomena at work relate to electrochemistry. These models have the advantage of being precise but are generally more complex and heavier in term of power calculation. A second family includes Analytical models. And the last family includes the models which describe the electrical behavior of the battery, which are the equivalent electric models.

Considering the other different approaches in the literature, we can suggest fractional order model is a mathematical representation that is justified for two main reasons:
- It allows the physical behavior of the cell to be well modeled because the same types of transfers are obtained using simplified electrochemical models.
- It is more precise than the other models' types, with an equivalent computational complexity.

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