

# TWAICE

## LFP IN ENERGY STORAGE

Why LFP batteries are playing an increasing role in energy storages and the implications of this on battery analytics

### WHITEPAPER

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## / INTRODUCTION

Lithium-ion batteries are an integral part of the transition to renewable energy, both for the automotive sector's transition to green mobility, and for the transition to generating electricity from more reliable and sustainable technologies. As renewable energy sources such as solar and wind are intermittent and therefore unreliable power sources, energy must be stored for certain periods of time. Technologies are required to stabilize the grid by ensuring that energy is released into the grid or removed from the grid when necessary.

Two major lithium-ion technologies are currently used in the field of stationary energy storages: NMC (Nickel Manganese Cobalt) and LFP

(Lithium Iron Phosphate). While people often speak about NMC and LFP cells, this naming describes only one half of the active materials in the cells. NMC and LFP refer to the cathode material of the cells. The anode part is often neglected as it usually consists of graphite in both cases and therefore does not need a further distinction. The set-up of lithium-ion batteries is explained in more detail below.

NMC is currently the most mature existing technology, and it is therefore widely used, especially in the automotive industry due to its beneficial specific energy and ideal combination of reasonable lifetime, safety, and reliability.

## / WHY ARE LFP CELLS GROWING IN POPULARITY?

LFP cells can be disadvantageous in terms of the specific amount of energy they can provide, meaning that an LFP battery with the same energy content as an NMC battery can weigh up to 25% more. However, this disadvantage does not apply to stationary energy storages, for which the size of a battery is less relevant. Integrators and owners of energy storages benefit from lower costs - according to [Bloomberg](#), LFP cells cost up to 20% less on cell level - and improved sustainability, as fewer toxic materials are required to produce the batteries and conditions for collecting the raw materials

are better. LFP cells are additionally safer and have longer lifetimes.

While most publications on the different cell technologies mostly concentrate on the above-mentioned aspects of safety, lifetime, or specific energy, one key aspect is often neglected: battery analytics and control.

LFP batteries come with a unique set of challenges in terms of battery analytics and operation. So, let's dive a little bit deeper.

## / WHAT IS BATTERY ANALYTICS ABOUT?

Let's look at it from a broader perspective. Proper state estimation of batteries is of the utmost importance in all cases where batteries are used, and that's why we at TWAICE bring battery analytics to the next level. You can only operate your energy storage to its full extent and keep your storage and therefore investment safe if you know accurately in which condition your storage is in.

To pick just one example for state estimation, let's talk about State of Charge (SoC). State of Charge describes how much charge is left in your battery to provide grid services, such as

frequency regulation or arbitrage. Figure 1 gives a schematic depiction of SoC explained, with a mostly depleted battery on the left and a fully charged one on the right.



Figure 1: State of Charge

## / WHY IS STATE OF CHARGE ESTIMATION IMPORTANT FOR ENERGY STORAGE

Proper SoC estimation is vital for stationary energy storages, as they fulfil important tasks such as emergency power generation in hospitals or grid stabilization. Consequently, improper state estimation, for example assuming an 80% SoC while only having 60% left, can have profound consequences in many ways and can cause safety issues and economic losses due to non-reliable storage operation. Not being able to deliver promised energy as grid service can lead to high fines or even permanent exclusion from grid service markets.

### / How state of charge is usually estimated

To estimate state of charge, there are a few major categories of methods:

- Charge throughput-based, called coulomb counting
- Voltage-based
- Filter-based, for example using Kalman filters
- Machine learning-based, comprising support vector machines, neural networks etc.

We will focus on the first 3 categories. But we shall keep in mind that machine learning models are simply different ways to capture, learn and later describe the behavior of a physical system called a battery. So, looking at it from a first principles perspective, every challenge arising from the physical properties of a cell also must be learned and solved by a machine learning approach as well. There is no shortcut here, only different ways regarding how to solve it.

### / Solutions for estimating State of Charge

Coulomb-counting

In this method, you take the assumption that it is impossible to measure current perfectly. This is due to sensor drifts caused by the thermal behavior of the sensors, limited sample rates etc. If we take a 100 Ah cell as an example and assume that when charged and discharged with  $C/2$  (discharge rate which causes a full discharge in 2 hours), we measure approx. 50.5 A on average instead of 50A. This causes an SoC error integration of 1%/full cycle. After only 20 cycles, the SoC already shows an error of 20%, meaning the storage can no longer be operated reliably.

#### Voltage-based methods

Again, voltages cannot be measured perfectly. But even more importantly, the open circuit voltage (OCV) changes with temperature and aging. In addition, there is a hysteresis behavior (dependence of the state of a system on its history), making it more unclear in which range of the hysteresis band the cell currently operates. With every load, the cell is further excited away from its relaxed state and depending on temperature and state of charge, relaxing back can take multiple hours. If we account for inhomogeneities in the electrodes which only very slowly diffuse back, sometimes it takes days or weeks. Combined with flat regions of the OCV (meaning a small change in OCV correlates to a big change in SoC), this renders accurate SoC estimation only based on measured voltages impossible.

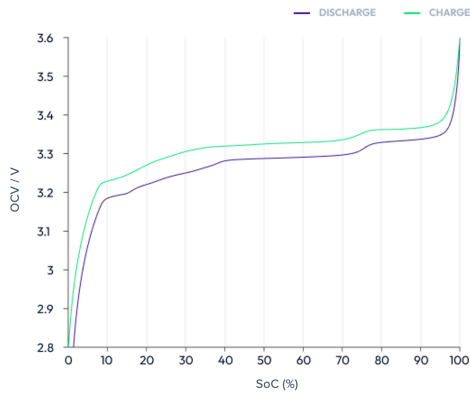


Figure 2: OCV & voltage hysteresis

### Kalman filter

So, what does this Kalman filter, that is mentioned in so many scientific papers, do? This third method, if we want to generalize it, is a sophisticated combination of the two methods to account for the issues mentioned above. Inside a Kalman Filter, a battery model is used to efficiently capture the battery behavior with state of charge and temperature dependency, hysteresis behavior, relaxation times etc. If this model would work perfectly well, combined with perfect sensor readings, we could always subtract the modeled dynamics from the real measured field data and would have our OCV, which could be mapped to our SoC again.

Unfortunately, there is no model existing today that provides 100% accuracy. Models differ in

their accuracy and reliability, but none of them can capture everything, especially when computational time and effort are taken into account. This is where Kalman filters come in. As mentioned, the Kalman-filter uses a battery model, e.g., an equivalent circuit model to combine it with uncertainties for a set of parameters. By this, theoretically, all model parameters as well as measured values can be accompanied by an uncertainty value accounting for errors or noise in sensor measurements, model parameterization errors etc. In each step, the Kalman-filter then corrects the estimation. Even though many types of Kalman filter exist, the first principle applies again, revealing the true challenge: How you tune your "noise Parameters" has the highest impact on your model accuracy.

### / Key takeaways

If we want to break it down into the simplest words, SoC estimation requires always knowing the state of your cells on the OCV (open-circuit voltage) curve. The OCV curve is the "passport" of the cell, showing you all essential information of the cell status at a glance. Either you always know exactly where you walked along your path (coulomb counting), or where you currently are (voltage measurement) or combine both with the knowledge that you do not know both for sure (Kalman filter).

We will now come back to the topic of NMC and LFP.

## / NMC AND LFP CHARACTERISTICS COMPARED

The insertion and extraction of lithium ions into and from the cathode material follows different physical paths in NMC and LFP cathodes. While NMC follows a so called “solid-phase-transformation” in which the entire cathode structure participates in the reaction, LFP exhibits a “phase-transformation” with a lithium rich and lithium poor phase in the cathode particles. As a simplified analogy, the behavior of the LFP cathode is comparable to boiling water. When heating up water, the water temperature will not increase above 100°C (at atmospheric pressure) until the entire liquid water has evaporated and the phase transformation from liquid to gas is finished. The structural differences between LFP and NMC reveal themselves as well when looking at their intrinsic safety property. As the oxygen atoms are more strongly bonded in the LFP structure, the material can withstand higher temperatures and generate less reaction heat when a thermal runaway occurs, thus, leading to higher safety & protection for thermal runaways.

But there is another aspect even more important if we look at it from the perspective of battery operation and battery analytics. The structural differences of LFP and NMC cause different shapes of the OCV of the respective cells. While NMC has a more monotonous slope of the curve, while of course showing different plateaus representing the different graphite stages, LFP comes with a very flat OCV especially in the region of 40 to 80 % SoC.

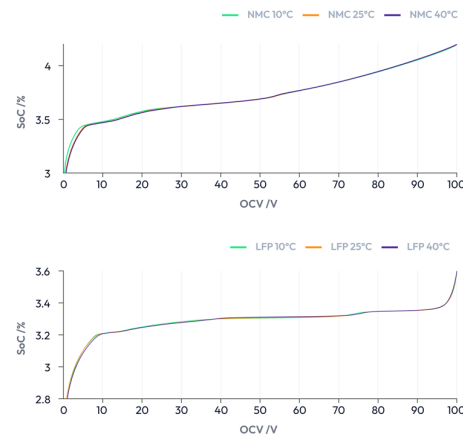


Figure 3: SoC of LFP and NMC cells

Let's assume you try to estimate SoC on a voltage-based basis: Already very small errors in voltage estimation can cause huge distortions on your SoC estimation. Coulomb counting also does not work as we have already discussed above.

Operating on a false SoC can have huge consequences for the operation of the respective storage, as discussed previously. It can result, on the one hand, in accelerated aging of the stationary energy storage system due to operation in unfavorable SoC ranges and, on the other hand, revenue losses and financial penalties due to unfulfilled contractual obligations.

This leaves us with the Kalman-filter-approach, but also this one becomes much more complex as little uncertainties in the hysteresis or the resistance parameters of the model also directly translate into higher uncertainties for the SoC estimation.

## / OUR ANALYTICS APPROACH FOR LFP CELLS

Estimating SoC for LFP cells therefore requires a unique combination of methods and resources. This combination comprises:

- High fidelity electric-thermal models accurately describe hysteresis. Relaxation is derived from initial parameterization in the laboratory.
- Deep battery analytics knowledge for Kalman filter tuning.
- Leveraging of field data to constantly keep track and update model parameters, such as impedance and resistance.
- Leveraging of field data, for example for artificial intelligence-based graphite stage detection as a reference and calibration tool.
- Combining with additional approaches, such as direct current resistance (DCR) & SoC correlation.

Utilizing field data to its full potential, the capacity estimation can be accompanied by a resistance or impedance estimation. As can be seen in the figure 4, the 30 s DCR shows a particularly significant relationship to the state of charge, especially when it comes to low SoC regions where operational risk is the highest as too low

SoC can cause unfulfillment of obligations of the storage operator.

Especially in the field of stationary energy storages, certain operation strategies such as intraday trading offer enormous potential as a storage is charged or discharged with an approx. constant power for several minutes. Combined with the flat voltage characteristic of the LFP cells, this offers a laboratory-like diagnostic pulse for our in-life analytics software to accurately determine the SoC for LFP storages.

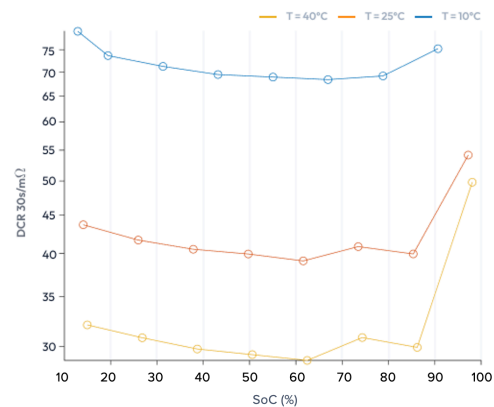


Figure 4: relationship between DCR and SoC

## / CONCLUSION: ESTIMATING THE SOC OF LFP CELLS IS A CHALLENGE

The major analytics challenge for LFP cells compared to NMC is the correct estimation of the SOC. The root cause originates from the flat OCV curve in which small voltage measuring errors result in a huge error in SOC determination. Operating battery energy storage under false SOC can lead to safety issues or result in economic impacts by not being able to deliver promised grid services and accelerated aging of the battery.

We combine multiple modeling approaches in a self-regulating manner and data from storages in

the field to maximize and constantly track the accuracy of the battery model. Additionally, we are increasing our lab capacity to examine common LFP cell types in our lab.

In case you face similar issues in operation, or you plan to build LFP-based battery energy storages, we are here to provide the best-practice LFP analytics to provide reliable SoC and SoH determination to provide peace of mind for your operators and trading strategy.



## / ABOUT TWAICE

TWAICE provides predictive analytics software that optimizes the development and operation of lithium-ion batteries. TWAICE's core technology is the digital twin – a software that combines deep battery knowledge and artificial intelligence to determine the condition and to predict battery aging and performance.

This makes complex battery systems more transparent, effective and reliable. As the leading battery analytics software for global players in the mobility and energy sectors, TWAICE is committed to increasing the lifetime, efficiency and sustainability of the products that power the economy of tomorrow.

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