Capacity Fade Modeling for Convex Optimization of Battery Charge/Discharge Schedules

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Abstract

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The use of electrochemical batteries to provide multiple system services can greatly increase the profit they are able to generate, which can help to offset their initial investment cost. By using battery scheduling optimizations, the optimal charge/discharge profile can be found for providing multiple services. However, the more frequently a battery is used, the more its energy capacity will degrade. This paper introduces a method for including and monetizing capacity fade costs into convex battery scheduling optimization so that they may be taken into account.
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Chapter 1: Background

Section 1: Electrochemical batteries and the power grid

In this chapter, the focus, significance, and relevance of this paper to the field of power system engineering are examined. This section introduces the importance of batteries to modern power grids and discusses how this importance will increase in the near future. The second section introduces the idea of battery scheduling and discusses the importance of incorporating accurate battery modeling into future power system simulations.

A discussion of the importance of electrochemical batteries to the power grid would be incomplete without also discussing the integration of renewable energy. According to a report by NREL, the amount of installed renewable energy sources around the world grew from 748GW to 1285GW between 2000 and 2011, an increase of 72%, which represents 22% of the total installed energy capacity during that time period [1]. Additionally, a separate report from 2012 prepared by NREL and Lawrence Berkeley National Laboratory predicts that wind energy installations will continue to experience cost reductions in the range of 20-30% through the year 2030 [2]. A similar trend has been seen for solar PV installations: at the time of the NREL report in 2013, PV systems had seen a substantial price decrease for a year and a half [1].

There are many positives to renewable energy sources, including but not limited to increased power generation capability, distributed and localized energy production, reduced carbon emissions, and potentially cheaper energy in the future.
However, the inclusion of intermittent sources like solar and wind creates a number of technical challenges. The stochastic and uncontrollable nature of these resources disturbs the power grid’s constant need for power balance between generation and consumption, as well as further exaggerates daily load fluctuations. A famous example of these problems is the California “duck curve” shown in the figure below, which predicts that as solar penetration increases, very sharp load changes will occur in the morning and evening as solar production ramps up and down, respectively.

![Figure 1: The Duck Curve produced by CAISO. [3]](image)

Both of the challenges listed above highlight well-known weaknesses for traditional generation resources (coal, nuclear, and to a lesser extent, natural gas),
as well as uncontrollable resources like wind and solar: their inability to store energy and limited ability to ramp power output up and down. However, these characteristics are strengths of batteries, which is why one of the most common applications of battery systems are for PV and wind plant smoothing, a service which keeps the power output of a solar or wind farm relatively constant over a period of time so that the rest of the power grid is insulated from the generation fluctuations. This service greatly increases the reliability of the connected power system by decreasing the amplitude of the power generation - consumption mismatches and simplifies the job of power system operators by making the net load more predictable.

While their large-scale use is currently uncommon, electrochemical batteries can also be used to shift load peaks to produce a less variable daily load profile (typical seasonal load profiles are shown in the figure below). This could be done by charging batteries at night and discharging them during peak hours, which would help traditional generators run at more efficient levels by decreasing the need for ramping power output up and down. This concept has been researched to ease the penetration of EV charging and better utilize demand-response, but it could be implemented with electrochemical batteries as well.
Figure 2.1 - Summer and Winter Daily Demand Profiles in 2010/11

Figure 2: Seasonal Load Profiles from National Grid (UK). [4]

If the predictions put forth by CAISO in the “duck curve” have any reputability, then the problems of increasing ramp rates and daily power consumption variability will need to be addressed in the near future. There are solutions for these problems that do not involve electrochemical batteries, like running conventional generators at inefficient levels, better utilizing demand response and EV charging, and changing energy consumption habits, but all of these options require sacrifices from multiple parties, mainly in the form of increased operating cost and decreased convenience. It is true that electrochemical batteries are still fairly expensive, with many grid-scale lithium-ion systems still in the $1000+/kWh range, but this price is expected to continue to decrease due to the increase in global electric vehicle purchases and integration of grid scale battery resources. However, the price of these batteries needs to be taken in context with
the flexibility services they can offer. Even at current prices, the services that a battery system can provide may be worth the cost due to the reduced strain on existing generation and control devices that a battery system would provide.

Section 2: Battery Scheduling and Modeling

The previous section discussed how batteries could be used to perform generation smoothing and help decrease daily load fluctuations, both of which are important technical challenges that will need to be addressed in the near future. However, there are other important services that batteries can provide to different users of the power grid. These services include, but are not limited to, transmission and distribution upgrade deferral, frequency regulation and energy reserve, and black start and contingency reserve. Some battery purchasers, such as utilities, may buy batteries for a specific purpose, like deferring the upgrade of an overloaded transformer or distribution line, while others may buy the battery as a general-purpose tool to help maintain power grid reliability. However, whatever the reason for the initial purpose of the battery, the reality is that it is very unlikely that the full potential of the battery will be constantly in use. As a result, there may be times of the year, or times of the day, when the battery may be available to provide other services.

Using a battery for multiple purposes has a number of advantages, but the primary one is the ability to make a profit from the battery instead of leaving it unused, which could help to pay off the initial investment in the battery. One of the ideas behind battery scheduling is that it allows an owner to determine whether or
not it is worthwhile to use the battery for other services. However, one of the main concerns surrounding this idea is that all actions by the battery will cause degradation to the battery components, which will lower the amount of time the battery can be used for whichever purpose led to its initial purchase. Additionally, different battery models have different power and energy ratings, dependent on the cell configuration, battery chemistry, and construction materials, which may make the implementation of a multi-purpose battery more difficult. Therefore, via battery scheduling optimizations, selling the available battery capacity for electricity or reserve purposes may bring more value to the battery and make the investment more profitable.

In order to determine whether or not a battery should be used for multiple purposes, or if it is financially feasible to buy a battery to participate in the reserve and electricity market, an accurate battery model and scheduling simulations are needed. Depending on the degree to which financial analysis is required and on the type of services that are essential, different degrees of simulation and battery modeling may be appropriate. For example, some scheduling simulations may require full transmission, generation, battery, and electricity market modeling, while others may only need a battery and simple market model. Additionally, smaller system models with low complexity may be able to accept more complex battery models while still maintaining a low simulation runtime. On the other hand, simulations with complex system models may need to keep the battery model as simple as possible for the same runtime constraints. The choice of the level of complexity to include in the model for various parts (transmission system,
generator models, battery models, electricity market, etc.) will depend on the
application of the battery and on the environment in which it will be used.

Determining the level of power system modeling (network, generation, and
market models) is fairly straightforward if the main purpose of the battery is
known. For example, a battery that will be used for transmission upgrade deferral
will require a less sophisticated power system model (grid, generators, market, etc.)
than a battery that would also participate in the electricity and reserve markets.
This is because a battery that is multi-purpose, and have interaction with electricity
and reserve markets, will need a more complete system model in order to
accurately determine the expected benefit from providing a variety of services. Once
the level of system modeling is known, the next step is to determine the level of
complexity for the battery model. For most power system simulations, convex
optimization will be used due to the number of time steps needed for simulation.
Therefore, the battery model itself will need to be convex, and preferably linear, in
order to fit into the existing optimization scheme. The most straightforward way to
build a convex battery model is to use experimental data to draw a linear or piece-
wise linear relationship between key independent variables, like power output and
state of charge, and capacity fade. This is the type of model that was chosen for this
paper, and which will be described in further detail in chapter 3.

If convex optimization is not a requirement, then more complex battery
models can be used. The reality of battery modeling is that the most accurate and
commonly used mathematical and first-principle models (both of which are
described in more detail in chapter 2) are based on nonlinear partial differential
equations due to the nonlinear nature of chemical reaction kinetics, particle kinetics, and thermal effects. Therefore, more accurate battery models can be used if convex optimization, and therefore computational runtime or long-term simulations, is not a priority. Mathematical and first-principle models also tend to be more generalizable and flexible to different scenarios, which are the main weaknesses of an empirical model. However, this weakness can be partially overcome by intelligently designing data-gathering and data-modeling experiments to produce a model that retains enough accuracy to be useful for the given application. This can be done by gathering experimental data on batteries running an output profile that will be typical of the behavior that will need to be modeled in the simulation and by using a battery that is technologically comparable to the one being used in reality.

In the context of determining whether or not a battery is suitable for a specified use, or for a combination of uses, an accurate capacity fade model is of paramount importance. It will allow for a more accurate calculation of life expectancy and for a prospective battery owner to determine exactly which uses the battery is suited to perform given a specified set of minimum performance and service requirements. Without a capacity fade model, the simulation is forced to make the highly erroneous assumption that batteries do not degrade or that all charge-discharge cycles produce an equal amount of capacity fade, both of which are highly inaccurate. The purpose of this paper is to show how a capacity fade model can be used to distinguish between different services and incorporate capacity fade modeling into battery scheduling simulations in order to determine the optimal operation of a battery.
Chapter 2: Introduction to Battery Modeling

Section 1: Electrochemical battery basics

Galvanic / Redox Reactions

A chemical reaction is a process in which a set of substances is transformed into another through changes in their chemistry. In a chemical reaction, the initial set of substances is known as the reactants and the final set of substances is known as the products. Reactions can be classified as either spontaneous or non-spontaneous; the classification of which depends on the energy state of the products relative to the reactants. In a spontaneous reaction, the energy state of the products is lower (and thus, more stable) than the reactants. This type of reaction is also known as exothermic because it releases energy in the process. In a non-spontaneous reaction, the reverse is true: the reactants have a lower energy state than the products (and are thus, less stable). This type of reaction is also known as endothermic because it requires energy to proceed. Additionally, in order for a reaction to be spontaneous, it also needs to be able to overcome its activation energy, which is the energy needed to start the reaction process. Therefore, not all exothermic reactions are spontaneous.

By harnessing these two types of reactions, different types of energy can be released and stored dependent on the direction in which the reaction is driven. This is the theory behind electrochemical batteries. When a battery is charging, electrical energy is used to drive the endothermic reaction, which in turn stores energy in the
form of chemical bonds. Reversely, when a battery is discharging, electrical energy is output as the exothermic reaction proceeds.

While all chemical reactions either release or store energy, not every type of reaction can be used to supply and store electricity. A class of reactions called reduction-oxidation is required because it involves the transfer of electrons from one substance to another. In these reactions, two substances with different reduction potentials are combined and the substance with the higher reduction potential (meaning it has a higher tendency to be reduced) is reduced (gains electrons) while the other substance is oxidized (loses electrons). These reactions are useful for creating electricity because the transfer of electrons from reactants to products (or vice versa) can be captured via an electrical circuit. This way, instead of the energy being given off as heat, the electrons perform work so that they are at the appropriate energy state when they recombine to with the active ions to make the products.

Battery cell components

Electrochemical batteries typically have three main components: an anode (negatively charged electrode), a cathode (positively charged electrode), and an electrolyte solution that conducts electricity. The figure below shows the typical layout of a lithium-ion battery and how the active material flows during charging and discharging. This diagram also shows how, while the electrons flow through an electrical circuit, the metal ions flow through the separator that separates the two half-cells and onto the opposite electrode. The separator is specially designed to
allow the metal ions through but resist the transfer of electrons so they move through the circuit instead of directly to the other electrode through the separator. In addition, the anode and cathode are specifically designed to bond with the active ions and facilitate the forwards and reverse reactions.

![Diagram of a lithium-ion battery](image)

**Figure 3:** Lithium-ion battery diagram. [5]

**Section 2: Lithium-ion battery introduction**

**Battery chemistries**

As discussed in the previous section, electrochemical batteries utilize a specific type of reaction, called a reduction-oxidation reaction, to convert chemical energy to electricity and vice versa. However, there are a great number of reactions
that can be classified as reduction-oxidation and not all of them are suitable for battery applications. In addition, not all reactions that are suitable for battery applications have the same performance. Different battery chemistries are generally classified and differentiated by the characteristics shown in the table below.

Although, when it comes to the commercialization of a battery technology, it is important to also consider the cost of production, which relies on the availability of the electrode material.

<table>
<thead>
<tr>
<th><strong>Battery characteristics</strong></th>
<th><strong>Definition</strong></th>
<th><strong>Unit</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Open-circuit voltage</td>
<td>Maximum voltage in the charged state at zero current</td>
<td>Volt (V)</td>
</tr>
<tr>
<td>Current</td>
<td>Low currents are characterized by activation losses, while the maximum current is normally determined by mass transfer limitations</td>
<td>Ampere (A)</td>
</tr>
<tr>
<td>Energy density</td>
<td>The energy that can be derived per unit volume of the weight of the cell</td>
<td>Watt-hours per liter (Wh/dm³)</td>
</tr>
<tr>
<td>Specific energy density</td>
<td>The energy that can be derived per unit weight of the cell (or sometimes per unit weight of the active electrode material)</td>
<td>Watt-hours per kilogram (Wh/kg)</td>
</tr>
<tr>
<td>Power density</td>
<td>The power that can be derived per unit weight of the cell</td>
<td>Watt per kilogram (W/kg)</td>
</tr>
<tr>
<td>Capacity</td>
<td>The theoretical capacity of a battery is the quantity of electricity involved in the electrochemical reaction</td>
<td>Ampere-hours per gram (Ah/g)</td>
</tr>
<tr>
<td>Shelf-life</td>
<td>The time a battery can be stored inactive before its capacity falls to 80%</td>
<td>Years</td>
</tr>
<tr>
<td>Service life</td>
<td>The time a battery can be used at various loads and temperatures</td>
<td>Hours (usually normalized for ampere per kilogram (A/kg) and ampere per liter (A/Lt³))</td>
</tr>
<tr>
<td>Cycle life</td>
<td>The number of discharge/charge cycles it can undergo before its capacity falls to 80%</td>
<td>Cycles</td>
</tr>
</tbody>
</table>

Table 1: Battery characteristics. [6]
There are many different battery chemistries, but the most widely used chemistries for rechargeable batteries are flow, lead-acid, nickel-cadmium, nickel-metal hydride, and lithium-ion [7]. Within each of these chemistries, there are various materials to choose from for the design of the electrodes, separators, and electrolyte solution. While the choice of battery chemistry itself has the largest impact on the overall performance of a battery, using different materials for the battery components can fine-tune the marketability in terms of performance, cost to produce, and cell size.

The table below shows the various characteristics for different battery chemistries. From this table, it is apparent why lithium-ion batteries have become increasingly popular in comparison to other chemistries. Of the five most popular chemistries, lithium-ion batteries have the highest energy density, the highest efficiency and the highest potential cycle-life. It also has a low self-discharge rate and does not suffer from what is known as the memory effect, which has the effect of lowering the energy capacity when a battery is charged after being only partially discharged.

However, one of the major disadvantages of lithium-ion batteries is their cost. Their development is fairly immature in comparison to other technologies, which means they have plenty of room to be improved, but are still fairly expensive to purchase due to the relative lack of large scale production.
Table 2: Characteristics and performance of commonly used rechargeable batteries. [7]

<table>
<thead>
<tr>
<th>Battery Type</th>
<th>Wh/kg</th>
<th>Cycle Life</th>
<th>Efficiency</th>
<th>Battery Costs ($/kW)</th>
<th>Battery Costs ($/kWh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow Cell</td>
<td>80</td>
<td>2000 - 10000</td>
<td>65%</td>
<td>2470 - 2600</td>
<td>300 - 350</td>
</tr>
<tr>
<td>Liquid Metal Battery</td>
<td>42</td>
<td>4500</td>
<td>90%</td>
<td>240 - 1200</td>
<td>30 - 150</td>
</tr>
<tr>
<td>Lithium-ion</td>
<td>185</td>
<td>2000 - 7000</td>
<td>90%</td>
<td>2970 - 4030</td>
<td>435 - 700</td>
</tr>
<tr>
<td>Long Life Lead Acid (LLLA)</td>
<td>41</td>
<td>4000</td>
<td>75%</td>
<td>2180 - 2900</td>
<td>370 - 520</td>
</tr>
<tr>
<td>Sodium Sulfur (NaS)</td>
<td>100</td>
<td>4500</td>
<td>80%</td>
<td>3900 - 4150</td>
<td>300 - 530</td>
</tr>
</tbody>
</table>

Section 3: Battery modeling

State of health (SOH) modeling basics

Electrochemical batteries are used for a wide variety of purposes, and it is important for all of them to have a way to accurately track the state of a battery. For all batteries, there are two main ways to determine the state of a battery. The first metric is called state of health (SOH) and is a measure of how much total capacity the battery has relative to the nominal, or initial, energy capacity of the battery. SOH is analogous to the term “capacity fade” as both refer to how the overall energy capacity of the battery changes over time. Like SOC, SOH is also measured on a scale from 0.0 to 1.0. Therefore, an SOH value of 1.0 means that the battery is new, while an SOH value of 0.0 means that the battery’s capacity is below suggested operating conditions and needs to be replaced. However, an SOH value of 0.0 does not mean that the battery will hold no capacity. General practice dictates that an SOH value of 0.0 corresponds to a battery that can hold 80% of its initial capacity [8].
The energy capacity of an electrochemical battery deteriorates for a number of reasons, all of which stem from the fact that the reaction within the battery and the materials used to support the reaction, are imperfect. Simply put, the capacity of a battery decreases over time due to the degradation of its components and the loss of active ions, which are the main participants of the redox reaction within the battery. However, there are a number of ways in which degradation and the loss of active material can occur. One of the main methods is through unwanted side reactions, which may or may not be reversible [9]. In a well-designed system, these unwanted side reactions would be limited by choosing active materials that heavily favor the wanted reduction-oxidation reaction. In many cases, this means that the energy required to perform the wanted reaction is much lower than the energy required to perform the unwanted side reactions. However, the fact that side reactions exist, coupled with the fact that the temperature of a battery will fluctuate during operation, means that side reactions are a reality of battery operation and as a result, the energy capacity of a battery will decrease with use.

While unwanted side reactions do play a significant role in capacity fade, the most prominent factor is the increase in resistance at electrodes [9]. There are different ways and different degrees of severity, dependent on the type of electrode being used, in which the resistance can increase in an electrode. In general, however, electrode resistance is increased due to some form of deterioration. This deterioration makes it more difficult for the chemical reaction to proceed, which causes fewer products to be made and limits the amount of energy that can be stored. An example of this deterioration is given by Zhang et. al., who studied the
cycle life of lithium-ion batteries with LiCoO$_2$ cathodes and carbon anodes by using discharge cycles of 1C, 2C, and 3C for extended periods of time [10]. They found that the LiCoO$_2$ cathode saw a much larger increase in resistance than the carbon anode over the period of 800 cycles and that the deterioration of the cathode was from an increased surface resistance caused by oxidation. It is also important to note that, in this context, cycle life is an analogous measure to SOH and capacity fade, and refers to how many cycles a battery can withstand before needing to be replaced.

*State of charge (SOC) modeling basics*

The second metric for determining the state of a battery is called state of charge (SOC), which is a measurement of the amount of chemical energy stored in a battery at a given point in time. It is scaled to the overall capacity of the battery, so that SOC is always between 0.0 and 1.0. A SOC equal to 1.0 indicates that the battery is fully charged and a SOC of 0.0 means that the battery is fully discharged. This is an important metric because it gives an estimate of how much energy is left in the battery, which can be used to determine how much longer the battery will run for a given power output.

However, predicting changes in SOC is not very straightforward. A common technique, especially in power systems, is to assume a constant efficiency for the battery at all points of operation. This assumption makes modeling SOC very simple, but it does not accurately represent how the SOC would change in normal operation. In actuality, changes in SOC are heavily dependent on a number of factors including, but not limited to, terminal voltage, current output, internal temperature, battery
chemistry, and internal resistance [11]. As a result, sophisticated, physics-based models are required to most accurately simulate the internal reactions and predict changes in SOC.

Further complicating the issue of predicting SOC is the fact that, during operation, the only observable quantities from the battery are the terminal voltage and the output current. From these two variables, it is easy to determine the amount of electrical energy being delivered, but it greatly increases the difficulty in determining the amount of chemical energy removed from the battery. This is another reason why physics-based models that simulate the internal kinetics and thermal effects of the battery are needed to most accurately predict changes in SOC.

For most batteries, there is a strong relationship between SOC and open circuit voltage, a value that relates to the equilibrium potential of the battery. However, as the name implies, open circuit voltage cannot be determined while the battery is in operation. Additionally, even if a battery were to be disconnected temporarily to determine the open circuit voltage, the measured value would not be accurate due to a principle called the recovery effect.

In essence, the recovery effect describes a phenomenon where the total amount of energy stored in a battery is not readily available due to the spatial location of active ions within the battery cell that prohibits them from being available for the reduction-oxidation reaction [12]. The figure below provides an intuitive diagram to explain the recovery effect. The figure shows how only the particles in contact with the electrode can be used for operation (either charge or discharge) and that this creates a spatial imbalance of particles. Over time, or after
the battery is given time to recover, the particles will even out so that more of them can be utilized for operation.

![Figure 4: Physical diagram for recovery effect. [12]](image)

Therefore, the recovery effect describes how, after a charge or discharge, the open circuit voltage will change and eventually equalize to a value that can be related to SOC. However, disconnecting the battery and waiting for the open circuit voltage to equilibrate is an unrealistic concession to make for the sole purpose of gaining accuracy in SOC prediction. An extension of the recovery effect is that if a battery is discharged under a higher current rate, the amount of energy delivered before the SOC is depleted will be less than if the battery was discharged at a lower
current rate. In order to deliver a comparable amount of energy, the battery will need time to recover so that the active ions can come to the surface of the electrode and undergo the reduction-oxidation reaction needed to release the chemical energy.

Temperature is also an important factor for predicting changes in SOC. Reaction kinetics are strongly tied to temperature, and as a result, the reduction-oxidation reaction within the battery is greatly affected by changes in temperature [6]. At high temperatures, degradation of materials or the activation of unwanted side reactions may occur, which greatly affects the overall health of the battery as well as the amount of stored chemical energy, which depletes the SOC. Conversely, at low temperature, there is less free energy in the environment to drive the reaction and active material becomes less mobile.

Internal resistance is another important factor for predicting changes in SOC, and is a quantity that combines many of the other effects already discussed, including temperature and degradation. In general terms, internal resistance is a measure of how different factors impede the progress of the reduction-oxidation reaction. The main factors that contribute to this effect are the current amount of stored energy, the ambient temperature, and the degradation of the electrodes and the separator. As the amount of stored energy decreases, reaction kinetics tells us that the reaction rate will naturally slow as the equilibrium is approached, which makes maintaining a constant current output more difficult and thus increasing the internal resistance. As discussed in the previous paragraph, temperature can affect resistance due to the decreased mobility of active material at low temperatures and
the increase in degradation and unwanted side reactions at high temperatures.

Finally, the degradation of the electrodes and separator naturally provides resistance to the movement of the active materials throughout the battery cell, which increases the measured internal resistance.

*Types of battery models*

When a battery model is made, it generally relies on experimental data to check the validity and tune the parameters. Typically, this is done by performing calendar and cycle life studies on a number of identical batteries that use the chemistry of interest. Over an extended period of time (generally long enough to deplete the SOH close to 0.0), the batteries are subjected to various current profiles at different temperatures to observe different behaviors and operating conditions. For example, Bloom et al. used three different current profile protocols to separately determine reference parameters, capture calendar effects, and determine the cycle life [13]. An example of one of these profiles is given in figure below, which shows the current profile for a 3% ΔSOC pulse. Bloom et al. also performed 6% ΔSOC pulse profiles, each of which were applied to batteries in a variety of temperature and initial SOC conditions.
In general, there are three main types of models that can be used to model SOC and SOH. The first type is called an empirical model. This type of model is often considered the least complex, as it does not attempt to model any of the physical or chemical effects within the battery. Instead, experimental data is gathered from battery tests that track changes in SOC and SOH through a variety of operating conditions. A relationship is then found between a few input variables (i.e. current and temperature) and the determined changes in SOC and SOH to come up with an equation to model the battery. The relationship that is found is generally one that gives the best fit to the experimental data. For this reason, the principal drawback to these types of models is their lack of generality. Because they are based on a specific set of experimental data, they may accurately model the specific batteries and conditions that were tested, but perform poorly when applied to different systems and different operating parameters.

Bloom et al. give an example of this type of model. An empirical model was developed from an accelerated study of Sony 18650 lithium-ion cells to determine
calendar and cycle life effects. The following equation was used to estimate the change in power capacity of the batteries over time.

\[ Q = A \exp \left( \frac{-E_a}{RT} \right) t^z \]

In this equation, \( Q \) represents the percent change in power capacity, \( A \) is an exponential parameter used to fit the experimental data, \( E_a \) is the activation energy of the reaction in J, \( R \) is the universal gas constant, \( T \) is the temperature in K, \( t \) is elapsed time, and \( z \) is the exponent of time. This model is empirical in nature because it uses a few simple parameters along with an adjustable constant \( A \) to fit the experimental data. In this case, Bloom et al. linearized the equation above and used the EXCEL function LINEST to determine the values for \( \ln(A) \), \( E_a/R \), and \( z \). A portion of the experimental data, along with the predicted quantities defined by the equation above, is shown in the figure below.

![Figure 6: Fitted curves for %increase in ASI dependent on time.][13]
The second type of model is called a mathematical model. In contrast to an empirical model, a mathematical model uses experimental data to model effects that contribute to the outcome instead of directly modeling the outcome. In the case of modeling capacity fade (changes in SOH), Ramadass et al. identified three main contributing factors: increase in resistance at electrodes, loss of the ability to bind lithium at the electrodes, and loss of active material in the cell [14]. In a mathematical model, the experimental data would be used to model these effects directly, which in turn would be related to capacity fade. This makes the model more complex, as it requires further research and knowledge of the subject to know which effects to model. However, the advantage of this type of model over an empirical model is its flexibility. Empirical models may fit the specific set of experimental data well, but mathematical models fit a wide variety of systems because they model the effects instead of the direct outcome. Doing so generally requires more knowledge of the system, which also means that more input variables and constants are needed, as well as more computation time.

The approach used by Ramadass et al. could be seen as a semi-empirical approach because it uses empirical data to draw relationships between specific effects and outcomes. There are other mathematical models that work in the opposite direction from this and attempt to simplify more complex first principle models, which are explained in the next paragraph. Some of the better-known models that fall into this category are the single particle model (SPM) and the 2D porous electrode model (P2D). Both of these models make assumptions about the configuration of the battery cell in order to simplify the first principle equations. For
example, the SPM model assumes that each electrode can be represented by a single
two-dimensional circular particle of uniform density [9]. This is not an accurate
assumption, but it does simplify the formulation and solution of the model. The P2D
model is slightly more complex and assumes that electrodes have multiple circular
particles within them, but that the battery cell only operates in two dimensions
instead of three. Again, this is not a valid assumption, but simulating battery
operation in two dimensions is much less computationally exhaustive than in three
dimensions.

The third type of model is called a first principles, or multiphysics, model.
This type of model is the most complex because it uses principal laws of physics and
chemistry to simulate the battery operation. This type of model is also the most
accurate, but requires the largest amount of input data and computational time.
Their complexity also makes them the most flexible because they simulate the
physics of the battery, which allows a model to fit many different battery
chemistries as well as simultaneously simulate SOC and SOH. In empirical models, as
well as most mathematical models, SOC and SOH are simulated separately because
they are based off of different sets of empirical data and require different
relationships and effects to fit the data.

There are different classes of models that fit into the category of multiphysics
models, and two of the most widely used are thermal models and
molecular/atomistic models. In general, a thermal model is one in which thermal
equations are incorporated into an existing mathematical or first principles model.
A common application of a thermal model is to add temperature effects into the P2D
model. This provides much more accuracy than the standard P2D model because reaction rates are highly temperature sensitive and batteries are subject to large temperature variations during operation [9].

Molecular/atomistic models differ from thermal models because they model the interactions of individual active particles, more specifically the process of intercalation into electrodes and passing through the separator. An example of this type of model is the Kinetic Monte Carlo method, which gets its name from its use of stochastic molecular interactions. These models are generally used to study battery operation in more detail than other models and are often focused on the movement of active ions through a specific part of the battery, which can help to optimize these materials and improve operation.

The choice of model depends on a number of factors, but Ramadesigan outlines an effective strategy for its development: “the simplest fundamentally strong model is developed that produces accurate enough predictions to address the objectives.” While this method may seem fairly obvious, the idea is to start with a basic model and continue to add complexity until the correct ratio of accuracy to computational complexity is achieved. Another important aspect is to pick a starting point that makes sense for the application. If accuracy is more important, it may be worthwhile to start with a mathematical model and build up to a first-principles model. On the other hand, if low computational complexity is more important, it may make more sense to start with a basic empirical model and add relationships and independent variables to increase accuracy to an acceptable level.
As with all forms of modeling, it is important to understand the limitations of the chosen model so that accurate conclusions can be drawn from its use. First-principle models produce the most reliable results, which means that many direct conclusions can be made. However, in the case of empirical models, it is important to understand which effects are not captured and understand how that will affect the results. Models of physical phenomena are very powerful tools that allow engineers and scientists to simulate complex systems, but at the end of the day they are still only models and will only partially match reality. As a result, the output of these models needs to be viewed through an educated lens forged from realistic expectations and a responsible understanding of the principles behind the model. If used properly, a model can be very insightful and have a large impact on the studied topic and its future research.
Chapter 3: Methodology

Section 1: Convex battery scheduling optimization neglecting capacity fade

In this section, the mathematics behind the convex battery scheduling optimization will be introduced. The modeling of capacity fade will be left out of this section so that the base optimization scheme can be better understood. There are a number of assumptions and simplifications that have been made in order to ensure that the problem is mixed-integer (meaning that the problem is made up of integer and binary variable), which will be discussed as they are introduced alongside the rest of the model.

The first equation shown below is the definition for energy output, which is the difference between energy sold and energy bought, where $f$ represents the efficiency of the battery. The objective function is shown next, which is a summation over all of the time periods of net income for two services, energy and reserve. However, the two services are monetized in different ways. For the energy service, the sale of energy is monetized, so multiplying the energy price by the energy output for that time period determines the income. For the reserve service, positive and negative power capacity is monetized, so the price for reserve power is multiplied by the absolute value of the power capacity sold to calculate income.

$$
E_{inj}^t = \frac{P_{en,dis}^t \Delta t}{f} - P_{en,ch}^t \Delta t * f
$$

$$
\text{maximize } \sum_{t=0}^{tf} (\lambda_{en}^t E_{inj}^t + \lambda_{res}^t P_{res}^t)
$$
The first simplification that must be introduced is that the price at each time point, and for each service, is a parameter, and is represented in the equation by $\lambda$. With this assumption, the model assumes that an individual battery has no effect on the market price and that it does not need to compete with other resources for the ability to sell energy and reserves, which will not always be the case in reality. However, assuming that the battery is a price taker means that the rest of the market, along with a variety of market participants and load profiles, does not need to be incorporated into the model, which greatly reduces the overall computational complexity and simplifies the development and analysis of the capacity fade model, which is the main focus of this paper. In addition, it means that the price profile used in the model will need to have a lot of variability so that different ratios of energy to reserve prices are included. This will allow the behavior of the model to be observed under a variety of market conditions.

The constraint on the power output by the battery at each time point is shown in the equations below. The constraints ensure that the power output for energy plus the reserve power output in both directions (up and down / discharge and charge) is within the power output limits of the battery. The power output limit, $P_{\text{lim}}$, is a parameter of the model, which will be different for various battery technologies, models, and manufacturers. Also note that a positive value of $P$ corresponds to power being injected. In addition to the two power limit constraints, the third equation constrains the amount of power supplied in each direction (up and down / discharge and charge) to be of equal magnitude, which signifies that the battery must provide symmetrical regulation.
Due to the assumption that the reserve service has no effect on the state of charge of the battery, there needs to be a constraint to prevent the battery from selling power capacity in a direction that is not feasible because of energy constraints. For example, if a battery is empty, then it is not feasible for the battery to provide up-regulation and if the battery is full, then it is not feasible for the battery to provide down-regulation. The following constraint is an attempt to solve this issue using a constant called the proportional factor, $k$, which is a parameter that determines how much energy capacity must be available for the battery to use in the direction in which reserve is being supplied. For example, if $P_{res,dis}^t = 50kW$ and $k = 0.5$, then there needs to be at least $k \cdot P_{res,dis}^t \Delta t = 0.5 \cdot 50kw \cdot 1h = 25kWh$ stored in the battery. There is also a previously unseen constant introduced in this equation, $c$, which represents the energy capacity of the battery and is used because SOC (state of charge) is a normalized value.

$$SO_{C_{min}} \leq SOC^t - k \cdot f \cdot \frac{P_{res,dis}^t \Delta t}{c}$$

$$SOC^t + k \cdot f \cdot \frac{P_{res,ch}^t \Delta t}{c} \leq SO_{C_{max}}$$

Lastly, the amount of energy stored in the battery needs to be tracked via the state of charge, which is modeled with the equation below. The second equation also limits the value of the state of charge to between its minimum and maximum values, because it is a normalized value.
\[ SOC^t = SOC^{t-1} - \frac{P_{in}^t \Delta t}{c} \]

\[ SOC_{min} \leq SOC^t \leq SOC_{max} \]

It is also important to note that, in this model, only the energy service impacts the state of charge. This is an assumption made in order to neglect the stochastic nature of signals that a battery would experience while providing reserve service, which would typically result in an unpredictable energy change during the time period. Therefore, this simplification means that the use of reserve service by the battery does not affect the amount of energy stored in the battery, but it is considered when determining the amount of power output by the battery, and thus the amount of capacity fade accrued by the battery over a given time period. This simplification is based off of the method used by CAISO in which the system operator restores the initial state of charge to each battery supplying the reserve service [15].

Those are all of the equations that are needed for the convex battery scheduling optimization problem neglecting capacity fade. In addition to the modeling equations, there are parameters that need to be defined, which include the price for each service at each time point, the efficiency of the battery, the capacity of the battery, and the power output limit of the battery.

Section 2: Development of convex capacity fade model

Choice of empirical model

As discussed in the second chapter, there are many different types of battery models, the choice of which depends on the application’s need for accuracy and
computational simplicity. For power system applications, low computational complexity is important because the capacity fade model will often be a small part of a much larger optimization scheme. Therefore, its contribution to the overall computation time should be minimal. This is not to say that accuracy is not important as well, but because we are not interested in the internal physics of the battery, it makes sense to use a model that is modular and can be built up until a complexity limit is reached.

Therefore, an empirical model was chosen because it allows the contributions and effects of different variables to be implemented separately. The model used by Johannesson et al. fits the requirements of power system applications because the data set can be approximated by a piecewise-linear function relatively well, which lowers the computation time and allows it to fit into an existing convex optimization scheme, and is only reliant on the average absolute value of power output over a given time frame, which can be easily calculated from existing variables and parameters in existing battery scheduling optimizations [8]. This model could also be extended to increase accuracy by gathering additional experimental data to simulate the effects of different variables like depth of discharge and temperature on capacity fade. This experimental data could then be modeled and implemented similarly to how Johannesson et al.’s model is implemented in this paper.

The model used in this paper is a piecewise-linear approximation of the data set used by Johannesson et al., which is shown in the figure below by the blue line. The data set is originally from a paper published by Wang et al., in which LiFePO₄
batteries were tested for capacity fade due to a number of variables including absolute value power output, temperature, and depth of discharge [16]. Wang et al. found that temperature and power output, especially at high values, are the most important factors for determining capacity fade, while depth of discharge has less of an effect. The figure below, from Johannesson et al.’s paper, has two main curves representing the number of expected cycles and the expected change in state of health for a given charge/discharge rate. The data from the change in state of health curve was used to determine the piecewise linear functions for the model in this paper.

![Figure 7: Change in SOH as a function of absolute value power output (represented by the thick blue line).](image)

_Monetizing capacity fade_

The existing model optimizes the battery output in order to maximize the profit made by the battery. Therefore, the final step in implementing the capacity
fade model into the base convex battery scheduling model is to monetize the capacity fade. In this implementation, the amount of capacity lost at each time step is tied to the initial cost of the battery. Therefore, a 1% change in state of health has a cost equal to 1% of the initial cost of the battery. This cost is then incorporated into the objective equation so that capital losses due to capacity fade are taken into account.

*Reserve factor*

While providing reserve service, a battery will follow control signals issued by the system operator, which tell the battery how much power to discharge at each time point. Due to this service’s stochastic nature, the average power output provided by the battery will not be known at all times and for all different batteries. Therefore, an approximation of the average power output for reserves, $\bar{p}_{res,dis}^t$ and $\bar{p}_{res,ch}^t$, for both charging and discharging, will need to be found to be used in the capacity fade model, derived from the amount of power capacity sold for the reserve service, $p_{res,dis}^t$ and $p_{res,ch}^t$. In this formulation, a constant called the reserve factor (represented by $r$) will be used to achieve this approximation using the equations below.

\[
\bar{p}_{res,dis}^t = r \cdot p_{res,dis}^t \\
\bar{p}_{res,ch}^t = r \cdot p_{res,ch}^t
\]
For example, if \( r = 0.05 \), \( P_{res,dis}^t = 100kW \), then the approximated average power output discharged for reserves, for time period \( t \) is 5kW, as shown by the equation below.

\[
r * P_{res,dis}^t = 0.05 * 100 = 5kW
\]

In this implementation, the reserve factor represents the average proportion of the power supplied for reserves that is used over the given time period. If historical reserve power output profiles are available, then the reserve factor can be found by finding the amount of energy provided in one direction (up or down / discharge or charge) and dividing it by the product of the power supplied for reserve and the time period. For example, if \( P_{res,dis}^t = 100kW \) and the amount of energy output for up regulation during that period is 5kWh, then \( r = \frac{5kWh}{100kW \cdot 1h} = 0.05 \). The figure below helps to illustrate this concept by showing an example of a regulation output profile (blue) along with the power supplied (purple) and the approximated average power output (red).
Figure 8: Example power output for regulation (blue) and the relationship between the approximated power output (red) and the supplied power (purple).

Section 3: Inclusion of battery capacity fade model

In order to include capacity fade modeling into the existing convex battery scheduling optimization model, some additional variables and equations are needed. First, the values for power output charged and discharged for both energy and reserve need to be used to determine the capacity fade at each time point, which is modeled via a three-segment piecewise-linear function. One simplification used for this calculation is that, given a large enough value of power output for energy such that the approximated power output for a given time period is unidirectional, the up and down regulation profiles will cancel each other out. This is not true for every time period, but it is generally true for a long enough time period. In order to calculate whether or not the reserve power outputs cancel each other out, the
absolute value of the power output for energy, $|P_{en}^t|$, is determined and then the approximated regulation outputs for both directions are centered around that value. For explanation purposes, the value of power output for down-regulation (charging) centered around $|P_{en}^t|$ will be represented by $P_{res,\text{min}}^t$ and the value of power output for up-regulation (discharging) centered around $|P_{en}^t|$ will be represented by $P_{res,\text{max}}^t$. The calculation for these values is shown below.

$$P_{res,\text{min}}^t = |P_{en}^t| - \overline{P_{res,\text{ch}}}$$

$$P_{res,\text{max}}^t = |P_{en}^t| + \overline{P_{res,\text{dis}}}$$

Once these values ($P_{res,\text{min}}^t$ and $P_{res,\text{max}}^t$) are centered around $|P_{en}^t|$, if they are both positive, then their power outputs cancel each other out. However, if $P_{res,\text{min}}^t$ is negative, then they will only partially cancel out, if at all. The equation below splits $P_{res,\text{min}}^t$ into its positive ($\overline{P_{res,\text{ch}}^t}$) and negative ($\overline{P_{res,\text{ch}}^{-}}$) components, only one of which will be nonzero. Therefore, if $\overline{P_{res,\text{ch}}}$ is nonzero, then the up and down-regulation components will not entirely cancel out, which is reflected by the second equation below, which shows that $\overline{P_{res,\text{dis}}^t}$ is cancelled out by the portion of $\overline{P_{res,\text{ch}}}$ that is greater than zero. The amount that is not cancelled out is then added to $|P_{en}^t|$ and set equal to the power output in each of three piecewise linear components ($P_{r1}^t$, $P_{r2}^t$, and $P_{r3}^t$) for the capacity fade model, only one of which will be nonzero.

$$P_{res,\text{min}}^t = \overline{P_{res,\text{ch}}^t}^+ - \overline{P_{res,\text{ch}}^-}$$

$$|P_{en}^t| + \left(\overline{P_{res,\text{dis}}^t} - \left(\overline{P_{res,\text{ch}}^t} - \overline{P_{res,\text{ch}}^-}\right)\right) = P_{r1}^t + P_{r2}^t + P_{r3}^t$$
The next equations introduce a binary system that is used to ensure that only one of the three segments has an associated power output. With these equations, only one of the three piecewise sections will have nonzero lower and upper limits. This is achieved by using the binary variables $r_1$, $r_2$, and $r_3$. For each of the three variables, a value of ‘1’ indicates that the section is ‘off’, while a value of ‘0’ indicates that the section is ‘on’. Therefore, given the first constraint below, only one of the piecewise sections can be ‘on’ at a time, which means that only one of the sections will have nonzero power output limits at a time.

\[ r_1^t + r_2^t + r_3^t \geq 2 \]
\[ p_{r_1}^t \geq 0 \times (r_2^t + r_3^t - 1) \]
\[ p_{r_1}^t \leq p_{r_1}^{lim} \times (r_2^t + r_3^t - 1) \]
\[ p_{r_2}^t \geq p_{r_2}^{lim} \times (r_1^t + r_3^t - 1) \]
\[ p_{r_2}^t \leq p_{r_2}^{lim} \times (r_1^t + r_2^t - 1) \]
\[ p_{r_3}^t \geq p_{r_3}^{lim} \times (r_1^t + r_2^t - 1) \]
\[ p_{r_3}^t \leq p_{r_3}^{lim} \times (r_1^t + r_2^t - 1) \]

Next, the following equations use the binary system defined above to calculate the capacity fade contributed by each section. The binary system is used again so that the capacity fade contribution is nonzero for only one section. The power output in each section is divided by the capacity because the model uses C-rate, which is a ratio of power output to total energy capacity, instead of power.

\[ \Delta SOH_{r_1}^t = (r_2^t + r_3^t - 1) \times \left( \frac{p_{r_1}^t}{c} \times r_{1\text{\textit{slope}}} + r_{1\text{\textit{int}}} \right) \]
\[ \Delta SOH_{r_2}^t = (r_1^t + r_3^t - 1) \times \left( \frac{p_{r_2}^t}{c} \times r_{2\text{\textit{slope}}} + r_{2\text{\textit{int}}} \right) \]
\[
\Delta SOH_{r3}^t = (r1^t + r2^t - 1) \times \left( \frac{p_{r3}^t}{c} \times r3_{slope} + r3_{int} \right)
\]

\[
\Delta SOH^t = \Delta SOH_{r1}^t + \Delta SOH_{r2}^t + \Delta SOH_{r3}^t
\]

Next, the capacity fade contributions for a given time period can be applied to the SOH variable.

\[
SOH^t = SOH^{t-1} - \Delta SOH^t
\]

Finally, the capacity fade for each time point (represented by \( \alpha_{cf}^t \)) can be monetized based on its initial cost (represented by \( \alpha_{init} \)), which results in a new objective equation. This full model can now be used to maximize profit in a given time period, while accounting for future losses by modeling and monetizing capacity fade.

\[
\alpha_{cf}^t = (SOH^{t-1} - SOH^t) \times \alpha_{init}
\]

\[
\text{maximize} \sum_{t=0}^{t_f} \left( \lambda_{en}^t E_{inj}^t + \lambda_{res}^t p_{res}^t f - \alpha_{cf}^t \right)
\]
Chapter 4: Results and Discussion

In this chapter, the results from the convex optimization model, which is described in detail in chapter 3, are discussed. Additionally, the impact that different parameters and design choices within the convex optimization model have on the results is discussed. The effect of these parameters is one of the main focuses of this chapter, as they will vary for different battery systems and implementations. The other focus of this chapter is to discuss the results of the base case and the implications that they have on the importance of capacity fade modeling. The following sections will introduce the results for the base case and discuss how the results change when different parameters are changed.

Section 1: Base Case Results

In this paper, the base case is defined to have the following characteristics. The energy and regulation service price data was pulled from the NYISO day-ahead energy and regulation markets for the week of June 1-7, 2014. Other sample weeks were used for comparison, but it was found that the general trend for different test cases was constant across the sample weeks. Therefore only one sample week, June 1-7, 2014, was used for in the final analysis.

The piecewise linear function is built from the data gathered by Wang et al. using 26,650 A123 Systems LiFePO$_4$ 2.2Ah cylindrical cells, which is shown in the figure below. The intersection points for the function were chosen to maximize the accuracy of the model within the operating region of the optimization scheme. The
cells are similar to what would be used in grid-scale deployments, as the chemistry is commonly used and A123 Systems makes grid-scale batteries using the technology. However, grid-scale deployments utilize a large number of these cells connected in series and parallel configurations, which introduces an additional dynamic of imbalance between cells. Therefore, even though the cells being used in real systems may be similar to the cells used for the capacity fade model in this paper, the data may be different from what would be gathered if a grid-scale battery were to be used as the test system. However, this data is not readily available and it would be much more expensive to perform capacity fade analysis on a battery system of that size.

Figure 9: Experimental data for capacity fade overlaid with three-segment piecewise-linear function.
The method of monetization of capacity fade is a very important design consideration as well. For this paper, the method used was to directly connect the amount of capacity fade to the initial cost of the battery. However, this may not be the best choice for all battery operators. With this method, the battery is treated as if it were on lease, in the sense that the battery operator pays for the depreciation of the battery. Therefore, this form of monetization will not maximize the profit that the battery could provide over its entire lifetime. Rather, it maximizes the profit that could be made for a given period while accounting for capacity fade as an operating cost. For example, it may be found that providing 500kW of power for energy provides an income of $1500 with a capacity fade cost of $50 for a given hour, and that providing 500kW of power for reserve provides an income of $1000 with a capacity fade cost of $10 for a given hour. Therefore, with this method of monetization, the battery schedule would choose to provide the energy service because the profit for energy ($1500-50=$1450) is greater than the profit for reserve ($1000-10=$900). However, from the viewpoint of maximizing the total amount of profit made over the life of the battery, this may not be the best decision because the energy service causes five times as much capacity fade as the reserve service ($50/10=5) without providing five times as much profit ($1450/900=1.61). Therefore, the method of monetization of capacity fade is an important design decision that may change depending on the situation and goals of the battery operator.
The battery energy and power ratings for the base case in this paper were chosen to be 500kWh and 1000kW, respectively. This represents a battery that is referred to as a “30-minute system” because it can discharge or charge all of its energy in 30 minutes. These values are reasonable because individual battery modules for grid-scale use tend to be on the order of a few hundred kWh and a 30-minute system is in the middle range of what is expected from a grid-scale battery, which generally range from 15-minute systems to multiple-hour systems. The efficiency of the battery is chosen to be 0.9486 for both charge and discharge, which represents a round-trip efficiency of 0.9. This is the quoted efficiency value by A123 Systems for their grid-scale systems, and is typical of other systems as well.

The proportional factor, which was introduced in chapter 3, is used to constrain the amount of regulation that a battery can provide in each direction based on how much energy is currently stored in the battery. This is a common constraint given by ISOs for providing the reserve service. For example, CAISO states in their guidelines that a reserve provider must be able to output their full power bid for up to 30 minutes [15]. Therefore, a proportional factor of 0.5 was chosen to represent that the battery must be able to discharge its power bid amount for half of the time period (which is one hour in this model).

The reserve factor, which was also introduced in chapter 3, is used to approximate the expected average power output for up and down regulation for a given time period and reserve power bid. As described in chapter 3, it can be found using historical regulation output data by calculating the amount of energy supplied in one direction (up or down) and dividing it by the potential amount of energy
supplied in that direction if the full reserve power bid was output for the time period. Since the data required to perform this calculation is not readily available in an academic environment, so a value of 0.05 was chosen as a reasonable value for the base case. Additionally, every ISO or region may have a different calculated value for the reserve factor and it could change depending on a number of other factors including season and time of day.

The last parameter of the model that has to be defined for the base case is the initial price of the battery. This information is also not readily available, and different battery technologies, deployments, and manufacturers provide a wide variety of prices. However, it is safe to make the assumption that a battery operator, in reality, would know the initial price of whichever battery they are modeling. For the base case, a value of $500/kWh was used. It is on the low-end for current battery prices, but using a lower value makes the model more applicable to the future (as battery prices, especially for lithium-ion batteries, are expected to continue to decrease) and setting a lower battery price leads to greater flexibility for the optimization program, which means that the effect of other parameters will be easier to analyze.

Now that the base case for the optimization model has been defined, the results of the model can be shown. The following figures show the results for two different optimizations, one that optimizes to include the price of capacity fade (labeled as CF) and another that does not take the price of capacity fade into account (labeled as NCF). The first two figures below show the power output profiles for each of the two optimizations, CF and NCF, respectively. The main difference
between the two is that in NCF, all of the power capacity is to provide reserve power, while in CF, the power output for reserve fluctuates and energy is bought and sold on the energy market at times. The reason for this difference is that in NCF, the battery is not penalized for having a high power output, so the optimization has chosen to run at its power output limit for the entire period (not including the charge at the beginning and discharge at the end). Additionally, one of the assumptions of the model is that reserve power output does not affect the energy stored in the battery. Therefore, without the cost of capacity fade, there is no operational cost for the battery to provide reserve in this model. On the energy market, the battery has an operational cost equal to how much the energy being discharged cost to buy. Therefore, it is scheduled much less often, if at all, when capacity fade is not accounted for.
Figure 10: Scheduled power output from 1-week optimized battery schedule incorporating capacity fade costs.

Figure 11: Scheduled power output from 1-week optimized battery schedule neglecting capacity fade costs.
The next figure shows the decline in state of health (SOH) for CF and NCF. Over the 1-week period, the schedule for CF causes the battery to lose around 0.3% of its operational health, while the schedule for NCF causes the battery to lose around 0.7% of its operational health, over twice as much. This difference in degradation is monetized in the next figure, which shows that in the NCF model, an income of $1612.62 was generated for the 1-week period, but the profit including capacity fade costs was -$77.04. On the other hand, for the CF model, an income of $1375.43 was generated, giving a profit of $681.88. This figure clearly shows the benefit and importance of taking capacity fade into account. Scheduling the battery output to include this cost resulted in less than a $300 decrease in income, but a net gain of $681.88 instead of a net loss of $77.04. However, it is also important to take these results in the context of the assumptions made for the model. Arguably the most important assumption for interpreting these results is that the battery did not have to compete to provide energy or reserve. Therefore, these results overestimate the income, profit, and capacity fade for both the CF and NCF models. Regardless of this fact, the benefits of the CF model in comparison to the NCF model are still valid as competition can be expected to affect both schedules equally.
Figure 12: Comparison of capacity fade between 1-week optimized battery schedules.

Figure 13: Comparison of income and profit between 1-week optimized battery schedules.
Section 2: Market Prices

The optimization model employed in this paper is designed to maximize the profit made by the battery through the performance of two services: energy and reserve. For this reason, the scheduling of the battery and the resultant profits are highly dependent on the market prices for the two services. In addition, each service has a different effect on the battery. Providing energy service requires discharging energy from the battery, which means that the energy to provide that service must be bought from the market beforehand. Therefore, in order to make a profit via the energy service, the gross income from the sale of energy must be greater than the
cost of the energy when it was previously charged and the cost of the capacity fade.

Additionally, the net income from providing the energy service must be greater than
the net income from providing the reserve service for that same time period.

However, these requirements are not true for the reserve service because power is
sold rather than energy. Therefore, the net income made from the reserve service
only has to be greater than the cost of capacity fade. Additionally, as with the energy
service, the net income from providing the reserve service must be greater than the
net income from providing the energy service. To simulate the expected variability
between prices for energy and reserve, prices from the NYISO day-ahead energy and
regulation markets were taken from June 1-7, 2014. The profile, which is shown in
the figure above, provides a reasonable amount of variability between the two
prices.

Section 3: Reserve Factor
In chapter 3, the reserve factor was introduced as a way to take into account the stochastic nature of regulation signals and approximate the average absolute value power output of the reserve service for a given time period. The choice of the reserve factor greatly affects the behavior of the model, as can be seen in the above figure. Therefore, the determination of this value is important to accurately predict the optimal schedule of the battery. If the reserve factor is set too low, it will over-predict the amount of profit made by underestimating the average absolute value power output of the reserve service, which in turn underestimates the amount of capacity fade and its associated costs. On the reverse side, if the reserve factor is set too high, then it will over estimate the cost of capacity fade, which will lower the
expected profits of the battery. Therefore, by not accurately determining the reserve factor, a battery operator could schedule the battery too aggressively or too conservatively. The determination of the reserve factor is described in further detail in chapter 3.

Section 4: Power Limit

Figure 16: Optimized profit for 1-week period dependent on power limit.

The choice of the charge/discharge power limit within the model is another important factor. However, for most battery modules, the battery manufacturer will have already determined the optimal power limit based on the battery’s chemistry, cell materials, cell configuration, and other construction and operational considerations. Therefore, one method for setting the power limit of the model
would be to set it equal to the rated power output limit. However, part of the purpose of this model is to take the effect of higher current rates on the degradation of the battery into account. Therefore, the power output limit can be set high enough to not be a constraint because the model will determine whether or not it is worthwhile to discharge/charge the battery at a higher rate. From using values in the base case, it was found that once the power limit exceeds 2C (1000kW in this case), it no longer interferes with the optimized schedule.

Section 5: Battery Cost

![Figure 17: Optimized profit for 1-week period dependent on initial battery cost in $/kWh.](image)

The battery cost used as a parameter for the battery schedule had a large impact on the results as well, which can be seen in the figure above. This has largely to do with the type of monetization used in this model, which directly tied battery
degradation to the initial cost of the battery. Therefore, a more expensive battery would see a larger cost of capacity fade for the same amount of degradation than a less expensive battery. This in turn creates a larger financial penalty for using the battery, which creates stricter criteria for determining whether or not an action is worthwhile in the context of making profit. Additionally, the figure above shows how, as prices of electrochemical batteries decrease, the expected profits will increase and the cost of capacity fade, at least by using this method of monetization, will decrease.
Chapter 5: Conclusions and Future Work

Section 1: Conclusions

The primary purpose of this paper is to demonstrate the importance of including capacity fade modeling into power system simulations that involve batteries. The results from the test case show that by neglecting the effects of capacity fade, the simulation is neglecting an expensive operating cost that may lead to the conclusion that a service is providing more profit than it would in reality. The inclusion of capacity fade costs takes the effects of battery degradation into account so that the battery scheduling optimization does not overestimate the value of providing different services. Additionally, the results from the test case show that there are ways to intelligently combine the scheduling of energy and reserve service to help reduce operational costs from capacity fade.

The secondary purpose of this paper is to propose a method for the inclusion of capacity fade modeling into existing convex optimization schemes. The proposed model, which is described in detail in chapter 3, uses experimental data from a capacity fade study of LiFePO₄ cells performed by Wang et al., which generated a convex relationship between capacity fade and power output, which is a key decision variable in any battery scheduling model. The proposed model contributes little additional complexity to convex optimizations, partly due to being approximated by a piecewise linear function, while still allowing for capacity fade to be calculated with a reasonable amount of accuracy by using experimental data on lithium-ion cells.
Section 2: Future work

The background information and modeling techniques used in this paper will help to bridge the gap in understanding between the fields of electrochemical engineering and power system engineering. Electrochemical engineering is concerned with the design and construction of electrochemical batteries while power system engineering is more concerned with the operation and benefits of electrochemical batteries. From the viewpoint of power system engineers, it is important to have a basic understanding of the electrochemistry used by the batteries in order to better understand how important state variables, like SOC and SOH, change during operation.

The future applications of the model proposed in this paper mainly involve its incorporation into more sophisticated and complete convex optimization models. These more complex simulations could include network models, generator models, market models, and load models, among others. In essence, the purpose of this paper is to introduce the concept of capacity fade modeling to the field power engineering research so that all simulations involving battery modeling can be more accurate. Capacity fade is a very important dynamic of battery operation and failing to include it will lead to inaccurate results and conclusions.

In addition to its inclusion in more complete systems, the model proposed in this paper could be redesigned to work in other battery operation environments and to analyze the effect of other services on optimal battery scheduling. For example, the inclusion of services such as black start, PV/wind smoothing, and
distribution upgrade deferral are all possible additions to this model that would not require much additional effort or complexity.
References


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