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Qualitative comparison of State of Charge prediction models for battery energy storage systems

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Abstract

Since increasing amounts of batteries are being introduced into the grid as flexible grid assets, they need to be incorporated into the prediction models for energy trading. However, batteries can be analytically approached in several ways. In this work, several battery models are compared. Afterwards, three models are implemented in a State of Charge prediction model. These models were validated with the help of a real battery at the University of Twente campus. Several measurements were done on this real battery, such as constant power (dis)charging and pulsed (dis)charging at several power levels. The accuracy of these three models is subsequently determined with validation measurements of the real battery. Since some of the models rely on a linear voltage prediction for the State of Charge prediction, two simple algorithms are proposed in order to avoid operation in the nonlinear voltage region of the battery. The work furthermore discusses on the role and application of these battery forecasting models for Balance Responsible Parties that are active on the Dutch electricity market.

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Nomenclature

Abbreviations

- API Application Programming Interface
- BMS Battery Management System
- BRP Balance Responsible Party
- DiBu Diffusion Buffer Model
- ECM Electrical equivalent Circuit Model
- EPEX European Power Exchange Market
- $KiBaM\,$ Kinetic Battery Model
- OCV Open Cell Voltage
- SoC State of Charge
- TSO Transmission System Operator

Physics Constants

e Euler's Number

Symbols

- ϵ Convergence Criterion
- C Capacitance
- E Energy
- I Current
- q Charge
- *R* Electrical Resistance
- t Time
- V Voltage

Chapter 1

Introduction

In this chapter, the technological background of the problem and the thesis structure are introduced.

1.1 Assignment Abstract

Since increasing amounts of batteries are being introduced into the grid as flexible grid assets, they need to be incorporated into prediction models for energy trading. However, batteries can be analytically approached in several ways, each with their own merits and applications. Since some of the models rely on a linear voltage prediction for the State of Charge, two simple algorithms are proposed in order to avoid operation in the nonlinear voltage region of the battery. The work also discusses on the role and application of these battery forecasting models for Balance Responsible Parties that are active on the Dutch electricity market.

1.2 Problem Background

Society is currently in the middle of an energy transition. This transition stems from global initiatives such as the well-known Paris Climate Agreement, as proposed during the COP 21 meeting. Since then, many of these conferences have taken place and they have helped society make a decision on what is necessary: reduce emissions of greenhouse gases into the atmosphere, in order to reduce the effects of climate change. The goal ultimately is limiting the effects of global warming to 1.5° Celsius temperature increase in comparison to the temperature as before the industrial revolution [1]. This temperature increase is heavily caused by the heavy emissions of CO₂ into the atmosphere. Historically, our energy is for a large share made from these fossil fuels. Therefore, society is looking for ways to produce energy from sources with less CO₂ emissions, and which are renewable on short term. Such sources are solar, wind, hydro, and others. By increasing the share of these sustainable sources in our energy mix, less fossil fuels are required, leading to reduced CO₂ emissions, but is also favourable since fossil fuels reserves are depleting rapidly. Therefore, in order to guarantee energy security, this transition to cleaner fuels is also required.

Where in the past energy was produced with conventional fuels and processes that emit a lot of greenhouse gases into the atmosphere, an ever increasing percentage of the energy mix is produced by means of sustainable and renewable energy sources, as can be seen from Figure 1.1. Besides this, society also has started using heavily more energy in absolute sense. Hence, replacing conventional

ways of producing energy with renewable sources will contribute immensely towards reaching the goals set in the Climate Agreement. Renewable energy sources still have their drawbacks however. Sources like solar and wind are subject to weather conditions. They are therefore less flexible than the conventional energy sources, which can be controlled in order to match supply and demand to one another. The consequence of this intermittency is that it is harder to match supply and demand to one another, which is vital to keep the local electricity grid in balance, by maintaining the frequency and voltage of the grid. When it is sunny, solar production peaks, but at these times, energy demand is often low. In the evening, demand will increase, yet the sun has gone down, meaning solar production is low.



Figure 1.1: Energy mix in the Netherlands over the last years [2]

Since it is vital to match supply and demand at any time during the day, there is a need to store energy, so that it can be used when it is required and production cannot satisfy the demand. This stored energy can then be used to complement the energy supply when there is a shortage of energy to supply the full demand, contributing to the stability of the local electricity grid. This way, the negative effects of the intermittency can be offset. To do so, forecasting is vital. With the use of forecasting, one can make a prediction on what energy flows will most likely occur in the near future. Forecasting is done with the use of computer models, which try to approach the real behaviour of assets such as e.g. batteries. Already, several battery models have been validated in literature. Hence, it is important to know the advantages and constraints of the available battery models, in order to choose the right model depending on the specifications of the given situation. Generally, these battery models are good at translating the linear behaviour of batteries, but have trouble representing the nonlinear behaviour. Therefore, it is important to realize that operation in the nonlinear region will result in deviations between the forecasting and reality. In order to keep the prediction as accurate as possible, the batteries can be controlled in a smart way such that they avoid operating in the nonlinear region, since this region is also often only found when applying deep-charge cycles, which generally is a mode of operation that is also to be avoided for battery health reasons.

It has been established in the previous paragraph that energy storage systems provide the flexibility needed to support renewable energy sources. In order to make good use of this flexibility, electricity also needs to be managed in a proper way to ensure performance of the local electricity grid within the boundaries. This can mean that there exists an electricity surplus or deficit at certain times. There always is a desire to match supply and demand on a national level too. Therefore, assets that produce electricity are only allowed to do so when there is an asset that requires this energy simultaneously, or in the case of batteries, one can make use of battery capacity to make sure a producer is able to produce electricity. Therefore, energy needs to be traded from producer to consumer.

In the Netherlands, this electricity can be traded on the European Power Exchange Market (EPEX), of which the Dutch electricity market is a part. Energy companies can buy and sell energy through this market. There are several markets for electricity, the forward market, the day-ahead market, the intra-day market and the balancing market [3]. The forward market is the very long term market, for the time frame of four years up to day before delivery, after which the energy enters the latter two markets, also know as the spot market. The day before delivery, the energy enters the day-ahead market. Here, the energy is traded for the next 24 hours in hourly blocks. This market is cleared at noon, after which the price per volume electricity is determined with a market clearing process for each hour. After this, the intra-day market opens, which is open up to 5 minutes before delivery of the energy. This market provides a possibility to trade electricity in quarter-hour intervals, providing the oppurtunity for market parties to respond to short-term deviations of their energy portfolio. All companies that trade energy have a requirement from the Dutch TSO, TenneT, to balance their portfolio's. These balance responsible parties (BRPs) therefore have to trade electricity on the spot market in case of a net nonzero volume in their portfolio. In order to calculate the prospective portfolios, many BRPs make predictions based on simulation models. These simulation models are used to predict the amount of energy that will be produced and the prospected demand, which together determine the amount of energy that needs to be corrected for on the market.

Battery energy storage, which can provide flexibility as established earlier, can be incorporated in this context in order to manage energy on all scales of the energy grid. As established earlier, forecasts are made based on computer models that cannot fully predict the behaviour of batteries. Therefore, a BRP wants to know what the constraints of the battery models impose in their portfolio forecasting, and based on these constraints, want to operate these batteries such that these constraints and prediction errors do occur as little as possible. Due to these errors, deviations from the prospected portfolio might occur, meaning the BRP does not fulfill the requirement of balancing their energy portfolio, resulting in fines from the TSO. For this reason too, it is important for the BRPs to have a reliable forecasting, including accurate battery models.

1.3 Thesis Structure

In Chapter 2, the assignment of this thesis described in more detail, together with the relevant research questions. Chapter 3 contains the relevant literature with respect to the aspects covered in the assignment description. In Chapter 4 the methodology and experiment is explained. Chapter 5 describes the results obtained from the experiment. Subsequently, Chapter 6 discusses the results, their validity, and provide an outlook on the socio-economic impact of battery energy storage in society. Lastly, Chapter 7 combines all results into conclusions and presents answers to the research questions posed, along with an outlook for possible future research.

Chapter 2

Assignment Description

This chapter describes the problem statement, and proposes the main research question along with several supporting sub-questions.

2.1 Assignment

As stated in the previous chapter, energy storage is a vital option to solve several problems at hand in the energy transition. Since electricity cannot be stored in its pure form, at least one energy conversion technology is needed [4]. Storing electricity can be done in several ways, yet batteries seem to be one of the most promising technologies [5]. However, batteries still face challenges in the field of smart grid technologies.

2.1.1 Digitization of Batteries

Many energy systems are supported by a digital model, that should mirror the performance of the physical battery system. These digital models are used to make predictions on the electricity and energy flows. Since batteries are technologically complex components, making a digital model of them is difficult and can be done in many ways, from simple to complex with increasing accuracy. However, detailed computations require more processing power and might also require more detailed information for the calculation to be executed. A range of battery models, used to estimate the State of Charge of the battery, has been validated in literature. The State of Charge is used to assess the amount of energy present in the battery. These digital models can also be applied performance evaluations of energy systems within portfolio's that are subject to balancing requirements. With a range of models available, it is difficult to choose the right model for each application.

2.1.2 Energy Market as Battery Management Control Signal

Since energy is a consumer product, there is also the need to analyse the impact that energy storage might have on the energy market. There is a spectrum of markets, using one or more of these markets as control signal for the energy storage system might lead to economic benefits for BRPs. The Dutch energy market consists of four sub markets, the forward, day-ahead, intra-day and balancing markets. Up to point of delivery, energy can be sold on either the forward or spot market. Therefore, depending on the battery model used, the maximum prediction horizon for accurate predictions plays a crucial role in the choice of market to trade on. In energy trading, a more accurate computer model is able to more accurately predict portfolio performance, and therefore can be used in order to optimize energy trading strategies for financial profit.

An assessment can be made based on increasing portfolio size as to which extent battery models can be used to act on the intra-day market. If batteries start taking up a significant volume in a portfolio, there might also arise a possibility to offer battery capacity as balancing reserve to the TSO, granted that batteries can fulfill the requirements the TSO has set. The integration of batteries in the energy markets also needs to be evaluated for in order to determine the desirable application of battery energy storage. As stated earlier, the battery models are a way of making forecasts of the expected battery behaviour. Therefore, the accuracy of the forecasts is vital. In order to make sure the batteries operate in the region where the prediction is most accurate, it is possible to smartly trade energy to prevent forecast deviations. For this application, one also wants to know the conditions for this deviation to occur, and find a suitable market to trade on in order to make up for this forecasting error.

2.1.3 Role of Forecasts

Battery models play a vital role in energy forecasting. The forecasts can lead to a difference between load and production in a BRP portfolio. This difference can be compensated for with an energy storage system in the form of batteries. This would lead to improved portfolio management for BRPs, making the portfolio more stable by having fully flexible energy storage assets. However, just like with the forecasting of solar yield or load profiles, the portfolio holder wants to have a significantly accurate battery model, that is also easy in use and applicable on a range of different batteries. The model should provide insight in the energy volume in the batteries, or the State of Charge. Therefore, in this work, several battery models are compared and applied, in order to find the strong and weak points of several promising battery technologies that are presented in detail in the literature review. The inaccuracies of the forecasts need to be compensated for either on the energy market, or by smart control algorithms. This way, the forecast can maintain its accuracy by making use of either smart control or the energy market as tool.

2.2 Research Questions

From the given assignment description, the relevance of modelling battery systems is clear. Hence, the main research question can be formulated as:

How can a suitable modelling technology be chosen to model a battery energy storage system?

In order to support this main research question, the following sub-questions are devised:

- What different modelling technologies are available?
- How can the decision for a suitable modelling technology be made?
- How can the battery model be applied to a fleet of batteries?
- How can battery energy storage models be applied smartly in energy trading?

Chapter 3

Literature Research

In order to determine the research gap, previously written literature is consulted in order to find relevant knowledge to support the executed research. Focal points will be different battery models, parameter research, energy markets.

3.1 Battery Fundamentals

Before one can understand different battery models, it is important to be aware of the fundamental properties of a battery, i.e. what properties define a battery? A battery is a device that converts energy between chemical and electrical form. An important sidenote for this is that this conversion should be (nearly) fully reversible. This means that a high amount of the chemical energy can be used again to produce electrical work [6]. The main components of a battery cell are the two electrodes, one positive and one negative, and the electrolyte. An electrolyte is a species that can conduct ions (both positive and negative), but does neither conduct nor contain free electrons. This in practice means that the electrolyte is a physical separator layer in the cell.

Batteries make use of electrochemical reactions. An electrochemical reaction is a reaction, in which the transfer of electrons goes from one species to another by the use of an electronic conductor. The transfer of electrons takes place from the oxidizing species to a reducing species, hence it is a oxidation-reduction reaction (redox). The overall chemical reaction consists of two half-cell reactions. In both of the half cell reactions, electrons play a vital role. In the oxidation reaction electrons are produced together with an cation, and in the reduction reaction electrons are used to form a pure metal. The reactions happen as the electrode surface, meaning that the compounds have to physically move to the electrode surface in order to chemically react.

3.1.1 Nonlinear Behaviour

A battery is subject to two important effects that cause nonlinear behaviour. The first is called the rate capacity effect, which is an effect caused by discharge current intensity, since with a high discharge current, less charge can be recovered in the battery [7], in combination with a lower voltage at high discharge currents due to lack of mixing of compounds in the battery. Since the reactions are electrode surface reactions, a high discharge current leads to a high reaction rate. This results in a low concentration of compound that can still electrochemically react near the electrode surface in comparison to a slow reaction rate (caused by a lower discharge current), leading to a lower potential and voltage. The second nonlinear effect, called the capacity recovery effect, occurs after a period of discharging, after which the battery has time to become more electrochemically stable, since the species in the electrolyte have time to get more homogeneously spread. Therefore, the concentration of the compound that can still electrochemically react will have time to increase near the electrode surface, increasing the potential and subsequently, voltage.

3.1.2 Open Cell Voltage

Since all the electrical equivalent circuits are represented with the open cell voltage as voltage source, it is vital to understand what this open circuit voltage (OCV) is. The open circuit voltage is the potential of the cell when no current is flowing. When no current is flowing there must be no load to the battery. The open circuit voltage follows from the electrochemical properties of the cell [6, 8]. It is heavily dependent on the material choice and concentration (due to the Nernst equation and the Butler-Volmer equation), and therefore can differ per battery. The open circuit voltage is also a (nonlinear) function of the state of charge of the battery. When a battery is loaded, mass transfer is required to bring the ions close to the reaction surface. Hence, there is a difference between the OCV and the closed circuit voltage, since when the battery is loaded, there will be mass transfer losses, ohmic losses due to conduction, and an overvoltage between the electrochemical reactions will occur (since now electrons can be transported).

3.2 Digitization of Physical systems

As is made clear in the previous section, batteries are complex assets. Therefore, modelling of these physical time-continuous systems using computers imposes a problem. Computers are classified as finite-state machines, and do calculations in discrete steps. In reality, electricity consumption is a continuous process, as is the behaviour of a battery energy storage system. A simulation is inherently made by using discrete time steps, and by making these time steps as small as possible, the resolution of data points increases in order to approach the behaviour of a time-continuous system.

3.3 Battery Models

Several of battery models have been devised in the last years, ranging from simple black box models, to intricate and complex chemical analyses, as done by Doyle et al. [9]. In this section, the most frequently used battery models are presented, after which each of these will be analysed and reflected upon. As a rule of thumb it holds, that the more complex the model, the more accurate it is in calculation, yet information is required to do so. In more complex models, nonlinear behaviour of batteries is captured better than in more simplified models.

Generally, models are used to calculated the state of charge of a battery. This value shows how much energy is stored in the battery as fraction of the maximum storable energy and can be mathematically described as in Equation (3.1), where E_{batt} is the energy in the battery, and E_{max} is the maximum storable energy. However, how the change in the State of Charge over a discrete step is calculated, differs in each model. The most applied method is Coulomb counting, where one measures the current applied to a battery, integrates this over time, in order to estimate the change in E_{batt} over time.

$$SoC = \frac{E_{batt}}{E_{max}} \tag{3.1}$$

3.3.1 Black Box Model

The most simple model of a battery is the black box model. In this model, the entire battery system is viewed as a single input/single output system, with a general round-trip efficiency. A schematic overview of the model can be found in Figure 3.1. This model can be used to make a back-of-the-envelope calculation on the magnitude of the energy flows, but it takes no (non)linear behaviour into account, and neglects other parameters such as battery voltage.



Figure 3.1: Schematic view of the black box model.

3.3.2 Electrical Equivalent Circuit Model

A more accurate model than the black box model is the widely used electrical equivalent circuit model (ECM). This model translates the battery to an electrical circuit containing voltage sources, resistances and capacitances. Such a circuit can be solved analytically in a way that is very common in the field of electrical engineering. It is adopted widely due to its relatively good accuracy and complexity [10]. Several different models are adopted in literature [11, 12], but the most used one uses the open circuit voltage of the cell as an ideal voltage source, together with a internal resistance, and has an open connection from which the battery terminal voltage is measured [13, 14, 15, 16]. Increasing in accuracy, several other methods are proposed, by the inclusion of capacitors, and by turning the electrical circuit into a Thévenin equivalent circuit [17], as is often done in electrical engineering.

The impedance of a battery is also nonconstant over the entire charge/discharge cycle of a battery [18]. Therefore, some simplifications are done in the model. A schematic overview of the model can be found in Figure 3.2. The model consists of the open cell voltage V_{OC} , and internal resistance R_{int} , and then a parallel circuit consisting of the polarization resistance R_{Th} and the transient capacitance C_{Th} that describes the transient charging behaviour. Based on this, an expression for the terminal voltage V_T can be derived based on Kirchhoff's voltage law (Equation (3.2)). In this equation, V_{OC} is the open circuit voltage, which is a function of the State of Charge. I_L is the current drawn from the battery at time t. Voltage V_{Th} is the voltage over the parallel connection of R_{Th} and C_{Th} at time t. By rearranging the expression, it can be written as in Equation (3.3).

$$V_{OC}(SoC) + I_L(t) \cdot R_{int} + V_{Th}(t) + V_T = 0$$
(3.2)

$$V_T = V_{OC}(SoC) - (I_L(t) \cdot R_{int} + V_{Th}(t))$$
(3.3)



Figure 3.2: Schematic drawing of the electrical equivalent circuit model [17].

3.3.3 Kinetic Battery Model

The Kinetic Battery Model, abbreviated as KiBaM, is a model proposed by Manwell [19]. It was first designed to model high capacity Lead-Acid batteries. In the model the battery is viewed in the sense of a two-tank model, one with a width of c representing the available charge, and the other with a width of 1-c representing the charge that is bound to the electrode, so that the total width of the tanks is equal to one. The tanks are connected with a valve that has a characteristic conductance, so that particles from the available charge tank can flow to the bound charge tank. This conductance is in theory equal to the chemical reaction rate, and is therefore often called k'. An overview of the model can be found in Figure 3.3. The total volume of the tanks is equal to the total amount of charge. The current regulator I operates in such a way that the current is constant during a time interval. The system can be described with the use of a set of differential equations, as shown in Equation (3.4).



Figure 3.3: Two-tank representation of the KiBaM Model [20].

The system can be described with the use of set of differential equations:

$$\begin{cases} \frac{di(t)}{dt} = -I(t) - k' \left(\frac{j(t)}{1-c} - \frac{i(t)}{c}\right) \\ \frac{dj(t)}{dt} = k' \left(\frac{j(t)}{1-c} - \frac{i(t)}{c}\right) \end{cases}$$
(3.4)

In this set of equations, i(t) is the amount of available charge at time t, I(t) is the current at time t, k' is the reaction rate constant, and j(t) is the amount of charge bound to the electrode at time t. In order to simplify the final mathematical equations, a new rate constant k is defined as:

$$k = \frac{k'}{c \cdot (1-c)} \tag{3.5}$$

By substituting Equation (3.5) into Equation (3.4), the system of equations becomes the following:

$$\begin{cases} \frac{di}{dt} = -I(t) - k(1-c)i(t) + kcj(t) \\ \frac{dj}{dt} = k(1-c)i(t) - kcj(t) \end{cases}$$
(3.6)

Differential equations like this can traditionally be solved by applying Laplace transforms [19], leading to the following system of equations:

$$\begin{cases} i = i_0 \cdot e^{-kt} + \frac{(q_0kc - I)(1 - e^{-kt})}{k} - \frac{Ic(kt - 1 + e^{-kt})}{k} \\ j = j_0 \cdot e^{-kt} + q_0(1 - c)(1 - e^{-kt}) - \frac{I(1 - c)(kt - 1 + e^{-kt})}{k} \end{cases}$$
(3.7)

In Equation (3.7) i_0 and j_0 are the initial value of available and bound charge respectively, and $q_0 = i_0 + j_0$, representing the total amount of charge at the initial time, which is equal to the initial battery capacity. In the KiBaM model, an important parameter is the difference between heights of the two species, often represented as δ , which is calculated with the formula shown in Equation (3.8). This parameter is able to capture the nonlinear behaviour of the battery [21]. This allows it to compensate for the rate capacity effect and the capacity recovery effect.

$$\delta(t) = \frac{j(t)}{1-c} - \frac{i(t)}{c}$$
(3.8)

From this, the unavailable charge $q_{n.a.}$, which is the charge that cannot be used for energy conversion, can be determined with the use of δ . With this $q_{n.a.}$, an estimation can be made for the State of Charge, as shown in Equation (3.10).

$$q_{n.a.}(t) = (1-c)\delta(t)$$
 (3.9)

$$SoC(t) = c - \frac{i(t)}{q_{max}}$$
(3.10)

3.3.4 Diffusion Model

Rakhmatov and Vrudhula proposed a different analytical model in 2001. It is based on the diffusion of ions in the electrolyte [22]. This model can be used to predict battery lifetime, but is difficult to apply when seeking State of Charge predictions. The authors use the term lifetime, but they actually refer the time to fully discharge a battery [23] under a constant discharge current. Therefore, under variable successive discharge speeds, calculating the state of charge becomes difficult, since a different time would have to be derived for each discharge speed. The model builds on the differential equations of one dimensional diffusion, as described in Fick's Laws of diffusion [24]:

$$-J(x,t) = D \frac{\partial C(x,t)}{\partial x}$$
(3.11)

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2}$$
(3.12)

J(x,t) equals the flux of species at time t at distance x, and D represents the diffusion coefficient. C(x,t) denotes the concentration of species at time $t \in [0, L]$ at distance $x \in [0, w]$ from the electrode [22]. In order to solve these formulas, boundary conditions have to be found. They are derived from the principles of Faraday's law, from which follows that at the left boundary (the electrode surface) the flux is equal to the electrical current i(t) flowing, and the flux at the right boundary is equal to zero. These conditions can be described as:

$$\frac{i(t)}{vFA} = D \frac{\partial C(x,t)}{\partial x} \Big|_{x=0}$$
(3.13)

$$0 = D \frac{\partial C(x,t)}{\partial x} \Big|_{x=w}$$
(3.14)

In Equation (3.13), v denotes the number of electrons, A the surface area of the electrode, and F is Faraday's constant. With the introduction of the boundary conditions, an analytical solution can be found. Using first a Laplace transform to transfer the equations to the complex frequency s-domain, followed by an inverse Laplace transform, an expression can be found to relate the time to full discharge to battery parameters α and β .

$$\alpha = \int_0^L \frac{i(t)}{\sqrt{L-t}} dt + 2\sum_{m=1}^\infty \int_0^L \frac{i(t)}{\sqrt{L-t}} e^{-\frac{\beta^2 m^2}{L-t}} dt$$
(3.15)

where $\alpha = vFA\sqrt{\pi \cdot D} \cdot C^* \cdot \rho(L)$ and $\beta = \frac{w}{\sqrt{D}}$. In the expression for α , C^* is the initial concentration for all x.

3.3.5 Diffusion Buffer Model

The Diffusion Buffer (DiBu) model is designed for accurate predictions of the battery State of Charge, yet easy integration within decentralized energy management systems [25]. The model can be used to predict the effect of a sequence of actions on the state of charge of a battery. It is also designed to be generally applicable, in constrast to other models, which are often tailored specifically to a certain type of battery [26]. The model describes the battery behaviour in four different states, charging, discharging, and an idle time after either charging or discharging. This implies that to determine if idling occurs after discharging. The DiBu model gives a comprehensive equation for the calculation of the state of charge at time interval [t, t + 1] [27]:

$$SoC_{t+1} = SoC_t + \frac{\Delta E_c - \Delta E_d - \Delta E_{loss}}{E_{max}},$$
(3.16)

in which ΔE_c is the charged energy, ΔE_d is the discharged energy and ΔE_{loss} is the energy loss, on interval [1,t+1]. However, in practice, a battery cannot both charge and discharge simultaneously, so at least one of the two parameters ΔE_c or ΔE_d is equal to zero at all times. The proposed model is set up in such a way that the losses due to charging and discharging are accounted for in the ΔE_c and ΔE_d terms, and secondary and tertiary losses, due to aging and non-charging related losses such as self discharge are neglected for simplicity. This means that the E_{loss} term is also equal to zero. In the model, the charging and discharging can be described with the help of the voltage and current vectors on the time interval [t,t+1], expressed as Δt :

$$\Delta E_c = \Delta E_d = \overline{V} \cdot \overline{I} \cdot \Delta t \tag{3.17}$$

In this equation, by convention, for discharging, $\overline{I} < 0$ and during charging $\overline{I} > 0$. By combining Equation (3.10) and Equation (3.17), the fundamental relation for State of Charge prediction in the DiBu model is obtained as in Equation (3.18), as a percentage of the maximum capacity E_{max} in Wh, based on the State of Charge at current time t. It calculates the future State of Charge by adding the expected change in State of Charge to the known State of Charge at the start of the discrete interval.

$$SoC_{t+1} = SoC_t + \frac{\overline{V} \cdot \overline{I} \cdot \Delta t}{E_{max}}$$
(3.18)

As can be seen from this equation, the change in State of Charge is dependent on the battery voltage during the process. The voltage in its turn, depends on what state the battery is in, and it requires an individual voltage relation for each of the states. The simplest state is the voltage when the battery has become idle after charging, since in this case, the battery voltage remains constant as charging has stopped [28]. The voltage in this state can be described as the voltage of the previous state, as shown in Equation (3.19).

$$V_{t+1} = V_t \tag{3.19}$$

There is a different expression required for the voltage prediction for idling after constant power discharge, in order to account for the voltage recovery effect of the battery. During idling after discharge, the battery has time to redistribute the compounds over the entire volume of the battery, increasing its potential, and therefore the voltage of the battery. This relation is described in the DiBu model with a first-order system approximation, as in Equation (3.20), which describes the relation between the initial voltage V_{t_0} at the beginning of the idling time (t_0) , and the starting voltage during the preceding discharge step (also the maximum voltage during the preceding step).

$$V_{t+1} = V_{t_0} + \left(V_{max} - V_{t_0}\right) \cdot \left(1 - e^{\frac{t-t_0}{\tau}}\right)$$
(3.20)

It is found experimentally that τ is not a constant, but also a function of the idling time. This relation is described as a linear function with two battery constants, β and γ , which are specific to the type of battery.

$$\tau = \beta \cdot (t - t_0) + \gamma \tag{3.21}$$

Substituting this equation into Equation (3.20), the final voltage can be calculating for a period of idling after a discharge period.

$$V_{t+1} = V_{t_0} + (V_{max} - V_{t_0}) \cdot \left(1 - e^{-\frac{t-t_0}{\beta * (t-t_0) + \gamma}}\right)$$
(3.22)

Now that the two voltage expressions for idling time have been derived, the expressions for the charging and discharging periods remain. From experiments it is observed that over time, voltage seems to increase linearly [26] during charging, with a slope that increases in steepness as charge current increases. From this, the relation as described in Equation (3.23) is found, with a battery parameter δ . The slope of the voltage is also dependent on this battery parameter.

$$V_{t+1} = V_t + \frac{\overline{I}}{\delta} \tag{3.23}$$

Lastly, the voltage during discharge has a fourth unique expression. From experimental discharging behaviour, two different parts can be identified [26]. At the beginning of the discharge cycle the voltage of the battery drops nearly linearly, up to a point where there is a sharp knee point in the voltage, after which the voltage drops steeply. The second part after the knee point, is has a very short time period, and is often an operation region that needs to be avoided. Operation in this region results in unwanted irreversible chemical reactions, leading to permanent capacity fading effects of the battery. Since this region of operation is to be avoided, the discharge behaviour is modelled in the DiBu model as only the first, more linear part. The slope of this linear approximation is dependent on the discharge current and the starting State of Charge, and is again subject to a battery parameter specific α for its type and capacity. The relation is expressed in Equation (3.24).

$$V_{t+1} = V_t + \frac{\alpha \cdot \overline{I}}{SoC_t} \tag{3.24}$$

For the DiBu model, it is important to find the battery constants α, β, γ and δ . These parameters can be found by doing charge and discharge tests for different currents. In the first iteration of the DiBu Model it was observed that the prediction accuracy decreased over large periods of time [26], which could be solved by periodically initializing the voltage and State of Charge of the battery by means of measurement. This inaccuracy was found to occur mostly during discharge periods, and was worse with higher discharge currents. Ideally, the measurements would therefore be done after a discharge step, effectively limiting the prediction length of the model to one charge/discharge cycle. In practice, a battery is placed with a Battery Management System (BMS), which measure current and voltage and can therefore determine the actual State of Charge.

3.3.6 Dualfoil Model

The most chemically and computationally complex model is perhaps the Dualfoil model. The model was proposed in order to find a way to model Lithium-polymer cells [9]. It is the most accurate model, however, it also needs a very large number of parameters to analytically determine the battery behaviour. A significant amount of these parameters are cell-specific (e.g. due to chemistry, size, geometry etc.) and are only known to the manufacturer of the specific cells. In practice, a lot of generalizations are required to apply this model due to lack of information. This constraint in turn leads to debatable application of the model. Besides this, making use of this model leads to a high amount of data use, as modeling for one cell might be a workable problem, yet if this model is to be applied to a fleet of batteries, the amount of data, calculation time, and computer processing time would get out of hand very fast. This model is in practice often used to validate the accuracy of other models when experimental data is not available [29].

3.3.7 Stochastic Models

The last type of battery models that is applied, is a the stochastic model, designed by Chiasserini and Rao [30]. It is a model that uses Markov chains to predict capacity of a battery, by viewing the battery as a state machine. From each state there is a certain probability to either move to a state of lower charge, to remain in the same state, or to recover one state of capacity due to idling. This model shows how to cope with the rate recovery effect by increasing the chance to recover capacity when in a lower state. However, this model is designed for situations in which the battery is discharged in pulses, allowing time to recover capacity after a discharge cycle. It is designed to show this recovery effect, and not necessarily to do State of Charge prediction. The model views the battery as a set of discrete states between 0 and N, where N is the assumed amount of charge that can be extracted under constant discharge rate. The step size between the states is equal to the amount of charge needed to send a packet of energy. It is assumed that the probability to decrease in charge level is q, and the probability to recover a charge state is expressed as:

$$p_i = (1 - q) \cdot e^{-\alpha(N - i)}, \tag{3.25}$$

where α is a battery constant related to the internal resistance of the battery and discharge rate. A smaller α leads to a higher recovery capability. If degradation of battery recovery capability is neglected, p_i is constant for all *i*. From these values, the probability to remain in the same state can be computed:

$$r_i = 1 - q - p_i \tag{3.26}$$

From this, a prediction can be made to see how many steps or time units it will take to reach the zero state, from state N:

$$n - N \ge 2k,\tag{3.27}$$

where k is the amount of right transitions, or the amount of times charge recovery has taken place. From these expressions, it is clear that this model is more suited for modeling the charge recovery effect in state machines, as opposed to State of Charge prediction.



Figure 3.4: Graphical representation of the Stochastic Markov model [30].

3.4 Battery Life Cycle

As batteries experience (dis)charge cycles over the course of the total lifecycle, they also are subject to degradation mechanisms. One of the most important degradation mechanisms is the loss of active material on both electrodes during active cycling. The deposition of Lithium has been related to decreased cell capacity and increased cell impedance [31]. The capacity tests have been executed over a large amount of cycles (500 up to several thousands) and it is noted that there is only a little decrease of cell voltage over the life time. Although this depends also partly on cycling depth, using non-deep cycling behaviour (discharging at most approximately 80 % of the battery, depending on the technology) can help extend the lifetime of the battery even longer. On a fleet of batteries, even a small percentage of capacity loss can lead to a significant total volume loss due to unavailable charge. Therefore, extending battery lifetime can lead to large cost reduction.

3.5 Energy Markets

As stated in Chapter 1, the introduction of large fleets of batteries also can have a lot of impact on the energy market. Since batteries are a fully flexible asset, they can be used in different markets, and also be used to bridge the gap between different markets by arbitraging [32]. The electricity market is a complex structure, consisting of several different market segments. These market segments are aimed at different timescales, and have different purposes. Making optimal use of the different market segments is crucial. The Dutch energy market comprises of 4 different market segments, the future, day-ahead, intra-day and balancing markets.

A party can trade energy freely on the first three of these. The balancing market is purely in place to give the Transmission System Operator (TSO) a portfolio of options to protect the balance of the grid, since this is the main purpose of the TSO. Parties can trade energy on the future market (up to four years in advance all the way down to approximately two days before delivery), the day-ahead market (up to noon the day before delivery), and the intra-day market (up to 5 minutes before delivery). An overview of the markets can be found in Figure 3.5. The future long-term market is more aimed at large consumers or producers who can afford to hedge prices for large volumes far ahead of time to guarantee a certain (often relatively low) price per unit volume, which helps their operations in both security of energy and financial sense.



Figure 3.5: Overview of the different energy markets in the Netherlands [3].

3.5.1 Day-ahead Market

On the day-ahead market, energy is traded up to 24 hours before the moment of delivery. The market closes at noon, after which the energy price is determined for each hour of the next day by means of market clearing principles. This price is generally seen as the "electricity price". However, a party only does a bid for a certain volume of energy, and therefore it is uncertain of the price they will have to pay for the volume traded on this market until the market clearing process is determined.

3.5.2 Intra-Day Market

On the intra-day market, BRPs have the opportunity to compensate for possible deviations from their portfolio handed in on the day-ahead market. On this market, prices are determined for every 15 minute interval, retroactively. Each minute a price is published, and based on the state of the grid, or the regulation activities required for the TSO to balance the grid, this price is determined. On this market, the BRPs are able to compensate for deviations in the demand/supply process. BRPs have a requirement to balance their portfolios, and if a deviation occurs with respect to the portfolio handed in for the day-ahead market, the party needs to trade energy on this market to restore balance in the portfolio.

3.5.3 Balancing Market

At the moment of energy delivery, the energy enters the balancing market. The role of this market is to provide the TSO with emergency volume that can be used when the grid stability is at risk of being jeopardized by large frequency deviations. This contracted volume has to comply to a lot of rules and prerequisities in order to be completely reliable for the applications TenneT wishes to see for. Since batteries are not a spinning reserve like flywheels with inertia, there needs to be certainty of the frequency delivered. Batteries therefore have extra requirements before they can be accepted in the role of Frequency Containment Reserve (FCR). The first requirement is the minimal power of 1 MW, with increments of 0.1 MW over the entire resource providing group, which can comprise of multiple batteries. The FCR volume is also activated based on an average frequency deviation, and it is not manually activated by the TSO [33].

3.5.4 Battery Implementation Strategy

If a BRP is able to incorporate battery systems into its portfolio, they might be used to gain economic benefits. Firstly, they can use this flexible energy volume to complement potential energy shortages in their production volume from the day-ahead portfolio, and while doing so the party can (partly) avoid buying energy on the intra-day market, for possibly high prices. Another possibility lies fully in the intra-day market. The Transmission System Operator (TSO), TenneT in the Netherlands, is concerned with maintaining the quality and balance on the electricity grid. They partly do so by stimulating a self-balancing market. BRPs should hand in their portfolios for the day-ahead market at noon each day of the year. They have an obligation to have balance in their portfolio, meaning that if they see a net result between supply and demand forecasting, they have to trade energy accordingly.

However, after this market closes, the energy enters the day-ahead market, which is used to trade energy based on short-term portfolio deviations, such as prediction errors that might be caused by unexpected weather circumstances. Based on the regulation state of the grid (if the TSO has to activate reserve supply or reserve demand to balance the grid) this price can be both positive and negative [33]. This price is determined by the TSO in such a way that there will be some self-correction in the market. In practice, BRPs are incentivised to deviate from their day-ahead portfolios if this contributes to grid stability. Should there be a net surplus of energy influx to the grid, a low, or maybe even negative price, will be set to encourage parties to buy this energy. Introducing fully flexible assets into the portfolio could lead to great benefits for the BRP. By combining predictive algorithms for the imbalance price such as proposed in literature [34, 35, 36, 37], energy can be traded when the prices are determined to be profitable for the BRP.

If energy prices are negative due to a large surplus of electricity inflow in the grid, buying this electricity both relieves grid stress, and actually results in net profit due to the negative price. If then this energy can be sold again in times of positive prices, profit can be made twice on the same volume of energy. However, in order to do so, it is important to have accurate predictions of the State of Charge of the batteries in the portfolio, to make accurate predictions on how much energy can be traded.

Secondly, the primary function of the batteries in the portfolio should be considered as well. If the battery systems are in place to supply energy to customers, a certain base volume should always be available in order to fulfill this primary function, and this volume should not be traded carelessly if the optimization criteria for the battery is economic profit. For this, also an accurate battery model is crucial, since if a BRP buys too much energy at a negative price, they will have to sell it back again on the imbalance market still at negative price, and possibly facing an additional fine imposed by the TSO for causing imbalance to the grid.

3.6 Conclusions

To conclude the literature research, it can be seen that several battery models have been devised already. These models are used to translate the physical continuous behaviour of batteries into a digital discrete twin. However, many of these models are purely used for specific battery types, and focus mostly on validating models. The validation of the battery models is often done with the use of regression models, since there often are battery parameters that are unknown. Therefore, options like Kalman filters can be used to reverse engineer this information. The validation of models is usually done by application on one battery of several battery technologies, disregarding the influence of large numbers of batteries. The found battery models each have their pros and cons.

The black box model is a heavy oversimplification of the battery and is therefore not very suited for implementation either. The electrical circuit model uses the laws of electrical engineering and its fundamental components to approximate the battery. It is often applied with slight variances, all trying to approximate the dynamic behaviour of batteries. It is also difficult to model the ECM voltage as function of State of Charge without experimental data.

The KiBaM model uses a two-tank principle with bound and available charge, connected with a valve that represents the reaction rate between the two tanks. This model can also be used to make a State of Charge prediction, when a relation between available charge and total charge can be found. The diffusion model is a model that focuses on the chemical dynamics of the battery. It is difficult to use this model to predict voltage, and would need some additions to make this work. It it therefore also deemed unsuitable for State of Charge prediction of large battery fleets.

The DiBu model can be used for State of Charge prediction once several battery parameters are determined, as the voltage can be determined with a finite state machine, after which the (dis)charge current can be used to relate this to the state of charge of the battery.

The Dualfoil model is the most accurate, but also the most difficult to implement. It has a very large number of parameters, some of which are specific for each battery cell. In order to justify using this model, all these parameters need to be known, some of which are not even known by the manufacturer. This would lead to huge calculations for increasing battery fleets, while only resulting in marginal accuracy results. Therefore, the Dualfoil model is also not classified as viable candidate for implementation.

The Stochastic models are primarily used for modelling the capacity recovery effect, which is not the scope of this research. Besides this, a probability based model is not very suitable for a situation in which the (short-term) future behaviour of the battery can be predicted. In practice, when a battery is placed, it is definitely possible to find the required parameters for the ECM, KiBaM, and DiBu model. Therefore, these models are deemed the most suitable for implementation. In conclusion, the most promising battery models for implementation are the Electrical Circuit Model, the Kinetic Battery Model, and the Diffusion Buffer model.

From the available literature, it is also concluded that incorporating the battery life cycle behaviour, e.g. battery degradation effects, is deemed outside the scope of the research. Due to the marginal influence, the availability of calibration possibility on batteries in the field, using complicated models to predict battery degradation seems unnecessary. In practice, it might be more useful to do regular checks on the battery fleet, to maybe assess voltage drops or temperature rise over the life time of the battery as State-of-Health indicators.

Lastly, from the literature research it is important to take into account the market that the energy of the battery fleet will be used on. The faster and more accurate the prediction model, the more suited a model is for energy trading close to moment of delivery. A fast algorithm can be used to trade closer to moment of delivery, on the intra-day market, where the electricity prices are generally higher than on markets further away from delivery. In order to be financially viable to offer the battery fleet capacity for the balancing market, the fleet has to adhere to the requirements. Since most home batteries are in the volume capacity of only few kWh, this would require a large fleet of batteries to be offered for balancing capacity, especially if a significant percentage of batteries will not be full at any given time. It is therefore determined that offering a fleet of batteries on the balancing market is not a viable option. The day-ahead market and the intra-day market, that together form the spot market, are deemed to most suitable when regarding prediction horizons.

Chapter 4

Methodology

To answer the research questions proposed in Chapter 2, several experiments are up. The results from these experiments will be used in order to support the answers on the (sub) research questions. This chapter introduces the experiments and their expected outcomes.

4.1 Experiment Goal

The goal of the experiment is to show the accuracy and applicability of several models found in the literature research. Since the main goal of the models is to determine the energy flow, a State of Charge prediction suffices for assessing the amount of energy in the battery. The experiment compares the found models to a physical battery, to see deviation of the models from reality. Depending on the occurring conditions of the prediction error, it might be important to see the impact that simultaneity of prediction errors has on the model accuracy. By comparing the actual energy volume to the expected energy volumes of the models, a conclusion can be made on which of the models is the most accurate for our application. The deviations in the models can be interpreted as a difference in energy performance between the real battery and the digital models. This difference represents an energy volume, which is either superfluous or shortage. From this, a strategy can be proposed in order to make up for a difference in energy volume between the digital model and the physical behaviour of the battery. To compare the models, first data needs to be used to find appropriate values for the battery parameters as described in Chapter 3. By using regression algorithms such as Support Vector Regression, Kalman filtering, or by using Linear regression, the value of these parameters can be found. These methods in a way determine the parameters so that the deviation from the physical performance of the battery is minimal. The battery used for in our case is the Slimpark KiWatt battery, located at the campus of the University of Twente. The most important information of this battery is displayed in table Table 4.1.

Table 4.1: Properties of the Slimpark Battery.

Property	Value	Unit
Technology	$LiFePO_4$	-
Capacity	30	kWh
Max Voltage	345	V
Max inverter Power	10	kW

4.2 Parameter Determination

With the use of experimental data of the KiWatt battery, the battery parameters necessary for the different battery models can be determined. This battery has been subject to testing cycles on charging, discharging, pulsed charge tests, and voltage recovery effects. The charging and discharging is done at several different constant power levels, and for the voltage recovery tests there has been variation in the time the battery was left to idle after a discharge cycle in order to assess the magnitude of the voltage recovery and the time needed to observe the voltage recovery. However, the experimental setup of the battery did pose some restraints on the data collection. The data that was logged from the battery was the State of Charge, pack current, stack voltage, the set point that was communicated from the user to the Battery Management System (BMS), the set point actually determined by the BMS, and the pack temperature. It was not possible to do measurements of the voltage on cell level with the experiment setup.

The communication to the battery management system worked with an application programming interface (API), which has a maximum amount of allowed calls to handle during a single day. To respect the health of the battery, the choice was made to not leave the battery in a fully discharged state overnight. The amount of calls allowed also put a restriction on the accuracy and the amount of measurement points that are obtained. Since the response time of the API also was slightly inconsistent, decreasing accuracy is expected in the found parameters that are time dependent. Lastly, the only way a set point can be passed on to the BMS is by assigning it with a certain power (both for charging and discharging), along with how long this power level should be maintained. Therefore, there is no possibility to discharge with a fully constant current, as the current fluctuates slightly along with the battery voltage and temperature. From these tests, the relation between the State of Charge and terminal voltage was determined experimentally. This relation is shown in Figure 4.1. The results of the constant power charge and discharge tests can be found in Figure 4.2.

The reason that the tests were done at constant power instead of constant current is the restriction in the battery management. It was only possible to give a set point for power and not for current. From these graphs, it can be noted that there is a clear nonlinear behaviour of the terminal voltage of the battery for both a very low State of Charge (SoC < 10%), and a high State of Charge (SoC > 95%). Operation in these regions are expected to lead to a prediction error in the models, since the models are the most accurate for the linear region of operation.



Figure 4.1: Terminal voltage as function of State of Charge for different charge powers.



Figure 4.2: Experimental data of charging and discharging the KiWatt battery at multiple constant power levels.

Next to this data, some tests were done to check the voltage recovery capabilities of the KiWatt battery. The battery was discharged, after which the battery was allowed to be idle for a certain idling period. During this phase, the battery voltage will rise again due to the chemical homogenization of the species inside the battery. However, the State of Charge will remain the same, since the available amount of charge does not change during the idling phase. The results of this experiment can be seen in Figure 4.3, which shows that there is only marginal voltage recovery present.



Figure 4.3: Voltage recovery as function of idling time.

4.2.1 Electrical Equivalent Circuit Model

For the electrical equivalent Circuit model, the most important parameters to determine are R_{int}, R_{Th} and C_{Th} . From [38], it is apparent that these parameters can be determined using pulsed charge and discharge cycle tests. These tests, just like the constant power tests, are also executed at several power levels for the pulses. Each pulse was applied three times. The measured data of the pulsed tests can be seen in Figure 4.4.



Figure 4.4: Voltage profile of the battery during the pulsed charge and discharge tests.

With the use of these results, the parameter values for R_{int} , R_{Th} and C_{Th} can be calculated. The internal resistance R_{int} can be determined by applying a charge current pulse to the battery. The initial terminal voltage increase is due to the internal resistance, which can then be calculated as follows:

$$R_{int} = \frac{\Delta V_{init}}{I},\tag{4.1}$$

where ΔV_{init} is the initial increase in voltage, and I is the current. The battery also shows more voltage increase after the initial spike, due to the effects of the parallel RC-pair. The resistance value of this RC-pair can be calculated using the following equation:

$$R_{Th} = \frac{\Delta V_{init} - \Delta V_{final}}{I} - R_{int}, \qquad (4.2)$$

where, ΔV_{final} is the final increase in voltage after the initial spike is finished. With this information, finally the value of the capacitance C_{Th} can be determined by making use of the time constant. Since an RC-circuit has a time constant, it is known from basic electronics that after a time of 5 times the time constant (also known as 5τ), the value has reached the final value within a range of less than 1 % deviation. This relaxation time can also be determined from the experiment. After this, the capacitance can be determined with the following equation:

$$C_{Th} = \frac{\Delta t_{relax}}{5 \cdot R_{Th}},\tag{4.3}$$

where Δt_{relax} is the time required to reach the final value within 1 % deviation, and R_{Th} is the resistance of the RC-pair. By using the available measurement data from the charge pulse tests,

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the parameters were found as presented in Table 4.2. All the values taken are the average over all the testing cycles.

Table 4.2: Determined parameters for the Electrical equivalent Circuit model.

Parameter	Value	\mathbf{Unit}
R_{int}	0.289	Ω
R_{th}	0.503	Ω
C_{th}	76.387	\mathbf{F}

4.2.2 Kinetic Battery Model

For the Kinetic Battery Model, the most important parameters to be determined are C, c and k. The nominal capacity C, expressed in Ah, can be approximated very well from the maximum capacity of the battery and the voltage. The other parameters, c and k', can be found using the results of the discharge and charge tests. Using the lifetime L, the time it takes to fully discharge the battery, in combination with the respective currents at certain discharge powers, an approximation of c and k' can be made using Equation (4.4) [39]. In Equation (4.4), W is the Lambert W function, which in mathematics represents the inverse function of $f(x) = xe^x$ [40]. Since from the discharge tests, multiple currents and lifetime values are known, using a least squares regression algorithm can be used to approximate the values for c and k'. The values that were determined can be found in Table 4.3.

$$L = \frac{C}{I} - \frac{1}{k'} \left(\frac{1-c}{c} + W \left(\frac{1-c}{c} e^{\frac{1-c}{c} - \frac{ck'}{l}} \right) \right)$$
(4.4)

Parameter	Value	\mathbf{Unit}
C	87	Ah
c	1.166	-
k'	0.986	\min^{-1}

Table 4.3: Determined parameters for the Kinetic Battery model.

Parameter Value Unit

4.2.3 Diffusion Buffer Model

For the DiBu model, there are four parameters that need to be determined, α, β, γ and δ . While looking at the equations that are used to describe the battery voltage for this model, it can be seen that α and δ can be found with a linear (first order) expression, but that β and γ are more complicated, as they are used in an exponential function. For the values of α and δ , a simple linear regression function can be used, and based on several measurement points an average value can be determined. For the values of β and γ , extra steps need to be taken. Since the function for the voltage idling after discharge contains a exponential component, an exponential regression function needs to be applied. This can be used to find the value for the time constant τ , after which the values for β and γ can be determined analytically.

Alpha α

Battery parameter α plays a role in the discharging phase of the battery. By making use of Equation (3.23), the value of α , can be analytically determined by making use of the charging data of the KiWatt battery. Since Equation (3.23) is a first order function, a linear regression algorithm should suffice in finding a value for α . However, the value of alpha can also be determined by

means of experimental results. Over a constant current discharge cycle, alpha is the slope of the discharge voltage over time. The results of the discharge tests of the KiWatt battery can be found in Table 4.4. Since a linear regression algorithm is used, it is also important to take into account the \mathbb{R}^2 value, which is a measure for the variance proportion of how good the slope is fit to the data. If there is very little variance, the slope is very consistent over the data, and the \mathbb{R}^2 value will be close to 1. This value therefore provides a measure of showing to what extent the dependent variable (in this case voltage) can be determined with the independent variable (alpha). The results of the regression seem to indicate non-constant behaviour of the parameter, this can be explained due to the fact that the tests were done at constant power instead of constant current. However, due to lack of time for intensive testing to compensate for the constant power restriction, the average of the found slopes is used as the final value for α .

Table 4.4: Slopes and \mathbb{R}^2 values for different discharge power levels.

Power (kW)	Slope	\mathbf{R}^2
2	0.0152	0.9083
3	0.021	0.8818
6	0.0472	0.9157
8	0.0571	0.9235
10	0.0652	0.9027

Beta β & Gamma γ

In order to find values for β and γ , Equation (3.22) is used. This function can be analytically rewritten to find a value for τ , as is done in Equation (4.5). These values can subsequently be used in a linear regression function to find β and γ , making use of Equation (3.21). In order to support this, an experiment was executed in which the voltage recovery effects were allowed to happen after a period of discharging. The battery was allowed to idle until the voltage no longer increased, as shown in Figure 4.3. The voltage at the beginning of the idling time t_0 was also logged, and is equal to V_{t0} , and the voltage at the end of the idling time (t), is equal to V_t . This was done for discharging after several discharge power levels. From this the value for τ can be used in a linear regression algorithm along with the value for $t - t_0$, in order to find suitable values for β and γ , respectively. In practice, the battery did only show marginal voltage recovery, even when the idling period was extended to over one hour. This is likely due to the chemical composition of the battery, since LiFePO₄ batteries do only show small voltage recovery effects [26]. This means that the parameters β and γ can be set to zero, in order to negate the effect of the voltage recovery.

$$\tau = \frac{(t - t_0)}{(1 - \ln(\frac{V_{max} - V_{t0}}{V_t - V_{t0}}))}$$
(4.5)

Delta δ

Parameter δ can be found by using Equation (3.24). This is a first order function just like with α , so a linear regression function also suffices in finding a value for this. Similar to the value of α , in a constant current charge cycle, the delta value is equal to the slope of the linear part of the graph. The test was repeated for the same 5 charging powers as for the discharging tests. The results can be found in Table 4.5. The results of the regression again seem to show non-constant behaviour for each of the parameters. However, due to the same constraints as for the determination of parameter α , also the average of the found slopes was used in the models for parameter δ . The used parameter values for the diffusion buffer model are given in Table 4.6.

Power (kW)	Slope	\mathbf{R}^2
2	0.0101	0.9199
3	0.0148	0.94
6	0.0254	0.9067
8	0.039	0.942
10	0.0397	0.8963

Table 4.5: Slopes and \mathbb{R}^2 values for different charge power levels.

Table 4.6: Determined parameters for the Diffusion Buffer model.

Parameter	Value	\mathbf{Unit}
α	0.04114	V/A
eta	0	-
γ	0	\min
δ	0.0258	A/V

4.3 Model Testing and Validation

Since the battery models are a digital approximation of a physical system, the results only provide context if they are compared to measurement data of a physical battery. Therefore, the voltage and State of Charge characteristics of the KiWatt battery, which is a Lithium Iron-Phosphate $(LiFePO_4)$ battery, are used. By using this data as input, the models can be validated, and missing parameters can be found by applying regression algorithms on the data set. The specifications of the KiWatt battery were presented in Table 4.1. In order to assess the accuracy of the models, all the models are tested against a devised load profile. In this test, the behaviour and prediction quality are compared against the behaviour of the KiWatt battery. From this an assessment can be made on the weak points of each model. Since in the previous sections the missing parameters and constants have been identified, now the models can be compared to experimental data of the KiWatt battery, in order to assess the accuracy of the implemented models. For this, a test case has been devised, for a set load profile containing charging, discharging, and idling phases. The load profile is shown in Table 4.7. One of the constraints of the test case is the set point, which is to be provided in Watts, meaning that the system is not to work with constant current profiles. In the test scenario, energy supplied to the batteries is taken positive, and energy taken from the batteries is assumed negative.

Table 4.7: Load profile used	l for the validation of	of the implemented	models.
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Step #	Profile	Power (kW)	Length (min)	Total Time (min)
1	Charging	3	60	60
2	Charging	8	60	120
3	Idle	0	30	150
4	Discharging	-2	30	180
5	Discharging	-3	30	210
6	Idle	0	30	240
7	Discharging	-8	30	270
8	Idle	0	30	300
9	Charging	10	120	420
10	Discharging	-10	120	540
11	Charging	6	60	600

4.4 Experiment Design

The experiment carried out focuses on the effects of the implementation of the different battery models. All battery models are expected to have their limitations, which impose accuracy issues in predicting State of Charge of the battery. This accuracy loss leads to a difference in actual stored energy and predicted stored energy. On a large fleet of batteries, simultaneity of prediction errors can lead to a significant deviation in the actual energy volume that is stored. If this is the case, it might be necessary to trade energy in order to make up for this deviation, which can happen in both upwards and downwards direction. This deviation can also be prevented by controlling the batteries in such a way that the batteries stay out of the inaccuracy region. Depending on the prediction window, imposed by the market, the specific market (day-ahead of intra-day) the energy is traded on also might vary. If energy has to be sold it might be more economically viable to do so on the intra-day market as prices are higher than in the day-ahead market, yet if energy has to be bought it would be less costly to know further in advance. Then, the energy can be bought earlier, often at a lower price.

Besides this, it is important to see that the problem is at its biggest when deviations occur in the same direction simultaneously. In the case the battery models are applied to a neighbourhood system with a large number of home batteries, it is expected that the behaviour of each battery is quite similar. After all, the neighbourhood shares the same weather, leading to similar PV performance and behaviour, and often neighbourhood houses have similar load profiles, resulting to similar battery sizes.

The energy forecasts rely on the accuracy of the battery models. In order to obtain the an accurate prediction, the prediction error needs to be minimized for each battery in the fleet. One way of doing this is by smartly moving energy around the fleet of batteries, to ensure the batteries do not operate in the nonlinear voltage region of the battery, since in this region the voltage prediction will be inaccurate. This happens because the voltage prediction relies on linear relations. Since the nonlinear region occurs at a very low and very high state of charge, the state of charge prediction from any of the prediction models, indicates that a battery in the fleet will reach the nonlinear voltage region. Therefore, after the state of charge prediction is made, it is possible to control the energy in the batteries in such a way that the prediction error of the batteries is minimized.

The state of charge at the initial conditions can be represented in vector form as $\mathbf{x}_i = (x_1, x_2, ..., x_N)$ for a fleet of N batteries. In similar manner a energy vector $\mathbf{E}_i = (E_1, E_2, ..., E_N)$ can be devised, containing the the change in State of Charge over the prediction. By element-wise addition of the initial state of charge \mathbf{x}_i and the change in state of charge \mathbf{E}_i , it is possible to represent the State of Charge prediction of the fleet of batteries as a vector $\overline{\mathbf{x}_i} = (\overline{x_1}, \overline{x_2}, ..., \overline{x_N})$.

From the state of charge prediction, a prediction error value P can be determined, based on the threshold of the linear voltage operation region. All these prediction errors are combined in the a vector $\mathbf{P}_i = (P_1, P_2, ..., P_N)$. The further the battery state of charge is from the linear voltage operation region, the larger the prediction error. By assigning energy exchanges over the batteries smartly, the algorithms try to iteratively minimize the total prediction error. In our case, this means minimizing the sum of the values in the prediction error vector \mathbf{P}_i squared, leading to the most accurate prediction possible.

The algorithms keep iterating as long as the reduction in error margin is still larger than the convergence criterion ϵ . The first algorithm tries to find convergence by finding the battery with the largest error and the smallest error, and equally divide the total energy of the two batteries. The pseudocode for this algorithm is shown in Algorithm 1.

The second optimization algorithm uses a slightly different approach. This algorithm is designed to move the minimal amount of energy per iteration, while maximizing the reduction in prediction error with this volume. It only determines how much energy necessary to reduce the largest prediction error, and moves this energy to the battery that has smallest error margin at the start of the iteration. Then it calculates the new error margin, and the algorithm keeps iterating until until a significant reduction of the error values can no longer be achieved. If this is no longer the case, convergence is reached. The pseudo-code for this algorithm is given in Algorithm 2. The hypothesis is that this algorithm should perform better, since per iteration less energy is moved, lowering the chance of inducing an error value in a battery that previously had no prediction error. Therefore, it is expected that this algorithm requires less iterations to converge, and that the total energy moved between over the process also is less in comparison to Algorithm 1.

To assess the performance of both algorithms, a test case is set up with a total of 1000 batteries. These batteries have been initialised with a random State of Charge, between 0 and 1. Both algorithms are fed this same vector of State of Charge values. A comparison is made on both the amount of iterations needed to reach convergence, and the amount of energy moved over the entire optimization process.

1:	function Averaging Energy Optimization($\mathbf{x}, \mathbf{P}, \mathbf{E}, N, X_{max}, X_{min}, \epsilon$)
2:	for $i \leftarrow 1, N$ do
3:	$\overline{\mathbf{x}_i} \leftarrow \mathbf{x}_i + \mathbf{E}_i$
4:	$ {\bf if} \ \overline{{\bf x}_i} < X_{max} \ {\bf and} \ \overline{{\bf x}_i} > X_{min} \ {\bf then} \\$
5:	$\mathbf{P}_i \leftarrow 0$
6:	else if $\overline{\mathbf{x}_i} > X_{max}$ then
7:	$\mathbf{P}_i \leftarrow \overline{\mathbf{x}_i} - X_{max} $
8:	$\mathbf{else \ if} \ \overline{\mathbf{x}_i} < X_{min} \ \mathbf{then}$
9:	$\mathbf{P}_i \leftarrow X_{min} - \mathbf{x}_i $
10:	end if
11:	$j \leftarrow 0$ (number of iterations to find optimal value)
12:	while $\Sigma \mathbf{P}_{i,j+1}^2 - \Sigma \mathbf{P}_{i,j}^2 > \epsilon$ do (iterative process)
13:	find \mathbf{i}_{Pmin} and \mathbf{i}_{Pmax}
14:	$\mathbf{x}_{min}, \mathbf{x}_{max} \leftarrow rac{\mathbf{x}_{max} + \mathbf{x}_{min}}{2}$
15:	$j \leftarrow j + 1$
16:	end while
17:	end for
18:	end function

Algorithm 1 Optimization algorithm to prevent prediction errors, using the equal splitting method

Algorithm 2	2 Optimization	algorithm	to	prevent	prediction	${\rm errors},$	moving	only	the	minimal
volume per ite	eration									

```
1: function MINIMAL ENERGY OPTIMIZATION(\mathbf{x}, \mathbf{P}, \mathbf{E}, N, X_{max}, X_{min}, \epsilon)
             for i \leftarrow 1, N do
 2:
 3:
                   \overline{\mathbf{x}_i} \leftarrow \mathbf{x}_i + \mathbf{E}_i
                   if \overline{\mathbf{x}_i} < X_{max} and \overline{\mathbf{x}_i} > X_{min} then
 4:
                          \mathbf{P}_i \leftarrow 0
 5:
                   else if \overline{\mathbf{x}_i} > X_{max} then
 6:
                          \mathbf{P}_i \leftarrow |\overline{\mathbf{x}_i} - X_{max}|
 7:
 8:
                   else if \overline{\mathbf{x}_i} < X_{min} then
 9:
                          \mathbf{P}_i \leftarrow |X_{min} - \mathbf{x}_i|
                   end if
10:
                   j \leftarrow 0 (number of iterations to find optimal value)
11:
                   while \Sigma \mathbf{P}_{i,j+1}^2 - \Sigma \mathbf{P}_{i,j}^2 > \epsilon do (iterative process)
12:
13:
                          find i<sub>Pmin</sub> and i<sub>Pmax</sub>
                          if \mathbf{x_{Pmax}} > X_{max} then
14:
15:
                                \Delta_{Emax} = \mathbf{x}_{\mathbf{Pmax}} - X_{max}
16:
                                \mathbf{x_{Pmax}} \leftarrow \mathbf{x_{Pmax}} - \Delta_{Emax}
                                \mathbf{x_{Pmin}} \leftarrow \mathbf{x_{Pmin}} + \Delta_{Emax}
17:
                          else if \mathbf{x}_{\mathbf{Pmax}} < X_{min} then
18:
19:
                                \Delta_{Emax} = X_{min} - \mathbf{x_{Pmax}}
                                \mathbf{x_{Pmax}} \leftarrow \mathbf{x_{Pmax}} + \Delta_{Emax}
20:
21:
                                \mathbf{x_{Pmin}} \leftarrow \mathbf{x_{Pmin}} - \Delta_{Emax}
                          end if
22:
                          j \leftarrow j + 1
23:
24:
                   end while
             end for
25:
26: end function
```

4.5 Conclusions

From the previous sections, it has become clear that with the use of experimental data, battery parameters for all models can be determined. For this, multiple charge and discharge tests were done. The KiWatt battery system at the University of Twente campus was put through several test cycles in order to determine the batteries parameters for all models. Several constant power levels were applied to determine parameters for the Kinetic Battery and Diffusion Buffer model. The diffusion buffer model parameters could not all be found from the constant power (dis)charge tests, therefore, an additional test was done in order to quantify the voltage recovery effects in the KiWatt Battery. To determine the parameters for the electrical circuit model, pulsed charge and discharge tests were done.

Since all models are expected to encounter inaccuracy issues when the battery is either in a very high State of Charge mode, or a very low State of Charge mode, two algorithms are devised to minimize this prediction error. The minimization of the prediction error is done by dividing the total energy stored in a fleet of batteries in such a way, that the batteries are kept out of the prediction error range. Two different strategies are proposed to do so, of which the first strategy is one in which the total energy of the batteries with the largest and smallest prediction error is equally divided over the two. The second strategy is only moving the energy volume that would reduce the prediction error to zero for the battery with the largest prediction error.

Chapter 5

Results

This chapter provides the results of the experiments as described in Chapter 4 and discusses their validity and outcomes.

5.1 Model Performance

In Chapter 4, the parameters of the models have been determined. Yet, the only way to assess the quality of the models is by comparing the predictions of each model to the actual behaviour of the battery. For this, the validation profile as shown in Table 4.7 was devised. The KiWatt battery was put though this sequence of discharge and charge cycles, and the profile was also applied to all three battery models. By comparing the accuracy of the battery models on both the State of Charge and voltage prediction, the overall quality of all models can be assessed. Since two of the models use a voltage prediction in order to determine the State of Charge, it is important to first assess the quality of the voltage prediction. The Kinetic Battery model is unable to make a voltage prediction, and is therefore not taken into account in the assessment for voltage prediction accuracy. The results of the validation can be found in Table 5.1, and are graphically shown in Figure 5.1.

Step $\#$	Profile	\mathbf{P}_{DiBu} (V)	\mathbf{P}_{DiBu} (%)	\mathbf{P}_{ECM} (V)	\mathbf{P}_{ECM} (%)
1	Charging	25.0	7.8	9.0	2.8
2	Charging	25.0	7.8	1.0	0.31
3	Idle	27.0	8.5	1.0	0.31
4	Discharging	29.6	9.4	4.0	1.3
5	Discharging	29.0	9.21	4.0	1.3
6	Idle	28.0	8.86	2.0	0.63
7	Discharging	28.2	8.98	2.0	0.64
8	Idle	28.2	8.29	4.0	1.3
9	Charging	20.0	6.15	2.0	0.62
10	Discharging	27.8	8.81	6.0	1.9
11	Charging	24.0	7.48	2.0	0.62

Table 5.1: Voltage prediction error at the end of each step of the validation profile.



Figure 5.1: Performance of the voltage prediction of each model over the proposed validation profile.

In the following comparison, State of Charge prediction behaviour is considered. Figure 5.2 shows the predictions of the State of Charge over the validation profile. The battery measurements started at 29% State of Charge, for which the initial conditions of the models were adapted. As can be seen from the validation profiles, the different models behave similarly, but with some different behaviour on some battery states. In order to determine the quality of each model, one may take a look at the error margin at the end of each profile step, in order to find an error pattern for each model. The results of this can be found in table Table 5.2.

The change in prediction error is calculated by dividing the absolute difference in State of Charge prediction and measurement by the measured State of Charge. This provides the relative prediction error due to this step. From this information, it can be seen that the Electrical Equivalent Circuit model performs the most accurate in comparison to the measured data, and that the diffusion buffer model performs the least accurate. The observed inaccuracy of the DiBu model is most likely due to the inaccurate voltage prediction, since this is a necessary step in the State of Charge prediction in this model. It can also be seen from the data that the KiBaM model performs poorly in the charging phases, where the prediction error increases. It is however accurate in the discharge phase.

5.2 Optimization Algorithm Performance

The optimization algorithms are designed to minimize the error prediction error over the battery fleet due to operation in the nonlinear voltage region. One algorithm approached this by averaging the energy of the batteries with the highest and the smallest prediction error, while the other algorithm only moved the minimal volume of energy required to reduce the maximum prediction error to zero. To assess the performance of both algorithms, a test case is set up with a fleet size of 1000 batteries. These batteries have been initialised with a random State of Charge, between 0 and 1. are fed this same vector of State of Charge values. A comparison is made on both the amount of iterations needed to reach convergence, and the amount of energy moved over the



Figure 5.2: Performance of the State of Charge prediction of each model over the proposed validation profile.

Step $\#$	Profile	\mathbf{P}_{DiBu} (%)	\mathbf{P}_{KiBaM} (%)	\mathbf{P}_{ECM} (%)
1	Charging	3.55	3.54	0.87
2	Charging	7.18	7.15	2.19
3	Idle	7.18	7.15	2.19
4	Discharging	6.51	6.48	1.72
5	Discharging	6.29	6.23	1.78
6	Idle	6.29	6.23	1.78
7	Discharging	2.13	1.79	0.65
8	Idle	2.13	1.79	0.65
9	Charging	2.04	2.04	2.04
10	Discharging	16.7	0.72	3.99
11	Charging	6.41	5.86	5.56

Table 5.2: State of Charge prediction error at the end of each step of the validation profile.

entire optimization process. Figure 5.3 shows the sum of the prediction error squared as function of the iteration number. It shows that the minimal energy algorithm finds convergence in fewer iterations, but it also reduces the error margin faster in comparison to the averaging energy . Next to this performance, it is also interesting to take a look at the energy volume moved during the optimization. In Figure 5.4 it can be seen that when applying the averaging algorithm, it takes a lot of time to actually start making progress towards the final solution, as the amount of energy transferred per iterations fluctuates significantly over the iterations. The minimal energy algorithm shows that for every iteration, less energy needs to be moved, and is therefore constantly and gradually getting closer to convergence. This also leads to a significant difference in total energy volume moved between both algorithms, which is shown in Figure 5.5. The minimal energy algorithm moves significantly less energy over the optimization process.



Figure 5.3: Prediction error as function of the iteration number for both algorithms.



Figure 5.4: Energy moved as function in each iteration for both algorithms



Figure 5.5: Subtotal energy volume moved over the optimization

Chapter 6

Discussion

This chapter discusses the results presented in Chapter 5, and also addresses the the socio-economic perspectives of the research. It discusses the possible applications of the research, its constraints, and opportunities.

6.1 Model Performance

In order to assess the performance of the developed models, one needs to keep in mind the overall goal of the models in the forecasting process, which is to make a forecast of the State of Charge over a certain period of time. Therefore, the total accuracy of this prediction weighs the heaviest. However, the voltage prediction step is a necessary step for State of Charge prediction with the electrical equivalent circuit and the diffusion buffer model. From the model validation (see Figure 5.1), it can be seen that the models in terms of voltage prediction are not the most accurate. The voltage prediction step in the diffusion buffer model reacts quite harshly during charging and discharging. The harsh behaviour of the voltage prediction means that the parameters for α and δ are not accurate enough. The origin of this inaccuracy might have to do with the measurement setup. The voltage measurements are done over the entire voltage pack, comprising of many cells. If the measurements would be redone over each individual cell, one might find a more accurate average value. In addition to this, the parameters β and γ were determined to be zero, for simplicity. However, the change in prediction accuracy over the idling step is zero. Therefore, the conclusion can be drawn that this simplification is justified for the KiWatt battery.

The Electrical Circuit Equivalent model implementation was based on the measurement data of the terminal voltage. This unfortunately defeats the purpose of the model, since it is a model that is used to predict the terminal voltage making use of the equivalent values for the electrical circuit components. However, from the measurement data, the relation between State of Charge and open cell voltage can be found, making use of the resistance and capacitance values found by regression. The only value necessary to determine the open circuit potential of the battery is the current, which is also measured from the KiWatt battery. For this model, the same footnote may be placed as done previously for the diffusion buffer model, since it might be the case this is inaccurate because of the measurements being done over the entire battery pack, instead of over the individual battery cells. For the model, the voltage was determined by a lookup table, containing the voltage as function of State of Charge data as measured for the constant power charge test at a power of 2 kW. This choice was made due to the resolution of measurement data. This is also most likely the reason that the ECM shows larger prediction errors at higher powers, since the voltage prediction is a little too optimistic. A higher discharge power would lead to a lower battery voltage at the same state of charge, due to the rate capacity effect, which is the effect caused by discharge current intensity, as with a high discharge current, less charge can be recovered in the battery [7], leading to lower voltages.

Since the Kinetic Battery model is unable to predict voltage, its application is limited to applications where voltage prediction is unimportant or impossible. The Kinetic battery model shows an increasing prediction error in the charging phase, but it seems to improve again in the discharging phase.

From the voltage prediction assessment results, as given in Table 5.1, it can be seen that the diffusion buffer has significant error margins in the voltage prediction. This means that the found parameters are inaccurate, which might be due to the measurement setup, since the measurement was done over the entire battery stack, instead of at battery cell level.

In order to assess the influence of this inaccurate voltage prediction, the Diffusion Buffer parameters are re-calibrated in an experimental way. By varying the parameters α and δ , one can modify the behaviour of voltage prediction during the charging and discharging. To do so, the two relevant formulas to make the voltage prediction in the DiBu model (Equation (3.23) and Equation (3.24)) are used. From these formulas, one can see that to let the voltage prediction act less extreme, α should decrease, whereas δ should increase. Due to the extreme nature of the voltage prediction error, the choice was made to change the parameter values in steps, a factor ten per step. The results of this can be seen in Figure 6.1. From Figure 6.1a can be seen that in the charging phase, the model behaves the closest to the measurements with where $\delta = 2.56$ in the charging phase since the voltage does no longer spike to the maximum voltage of the battery. In the discharging phase the model behaves the best in the situation where $\alpha = 0.4114$, since the the voltage change over the discharge step now is closer to that of the measured date. By combining the two improved values into one model, the total voltage profile behaves better than the original valued one, which can be seen from Figure 6.2a.



Figure 6.1: Voltage and State of Charge prediction for multiple values of α and δ .



Figure 6.2: Voltage and State of Charge prediction for the initial parameters and the improved parameters α and δ of the Diffusion Buffer model.

The improved diffusion buffer model can also be compared with the other two models, to see if the improved parameters made a significant difference in prediction accuracy. The results of this are shown in Figure 6.3 and Figure 6.4. It can be seen that improved diffusion buffer model perform significantly more accurate. This is confirmed when looking at the error margins of the improved diffusion buffer model in comparison to the original models. which can be seen in Table 6.1 and Figure 6.5. However, the ECM is still more accurate than the improved DiBU model in most of the steps of the validation profile. However, in the discharge phase, the improved DiBu model, performs better than the ECM model for this application. Next to this, it can also be seen that all models have a similar prediction error in the nonlinear voltage region of the battery (the end of step # 9), even the KiBaM model which does not make a voltage prediction.



Figure 6.3: Performance of the voltage prediction of each model over the proposed validation profile, including the improved DiBu model.



Figure 6.4: Performance of the State of Charge prediction of each model over the proposed validation profile, including the improved DiBu model.

Table 6.1: State of Charge prediction error at the end of each step of the validation profile, include	ling
the improved DiBu model.	

Step $\#$	Profile	\mathbf{P}_{DiBu} (%)	$\mathbf{P}_{DiBu,impr}$ (%)	\mathbf{P}_{KiBaM} (%)	\mathbf{P}_{ECM} (%)
1	Charging	3.55	1.30	3.54	0.87
2	Charging	7.18	3.73	7.15	2.19
3	Idle	7.18	3.73	7.15	2.19
4	Discharging	6.51	2.91	6.48	1.72
5	Discharging	6.29	3.17	6.23	1.78
6	Idle	6.29	3.17	6.23	1.78
7	Discharging	2.13	1.32	1.79	0.65
8	Idle	2.13	1.32	1.79	0.65
9	Charging	2.04	2.04	2.04	2.04
10	Discharging	16.7	2.02	0.72	3.99
11	Charging	6.41	1.14	5.86	5.56

6.2 Optimization Algorithms

Next to prediction errors due to operation in the nonlinear voltage region of the batteries, other inaccuracies also occur. One of these inaccuracies originates in the mode of operation of the battery. However, in order to integrate this into the optimization algorithms, some kind of relation needs to be found between the predicted current (or energy) that is applied to the battery and the expected error margin that this applied current introduces. This prediction error is also one that cannot be prevented, as opposed to the prediction error that would arise due to operation in the nonlinear voltage behaviour region, which is solved by preventing operation in this region with the use of the optimization algorithms.

When looking at the optimization algorithms, it is clear that the averaging model performs significantly less than the minimal energy transferring algorithm. This is in line with the hypothesis, and has several significant advantages. Moving less energy is first of all desirable, since transport of electrical energy goes paired with losses. To transport the energy from one battery to another,



Figure 6.5: Error margin in the State of Charge prediction of each model over the proposed validation profile.

the energy first needs to be converted from chemical to direct current electrical energy, then from direct current to alternating current, then transported, converted back to direct current in order to charge the other battery with the energy, being back at chemical energy. These three steps all induce losses. An DC/AC inversion step typically is around 98% efficient. Its counterpart, the AC/DC conversion, is even less efficient, stagnating at efficiencies of around 85-90%. This means that a significant amount of energy would be lost, in order to keep the voltage (and thus the State of Charge) prediction accurate. Next to this, the transport of energy requires a new charge/discharge cycle for both batteries, which goes at the expense of battery lifetime.

6.3 Energy Economics

As found in the literature research, energy can be traded in several market segments. In the context of this research it is important to take a look at when the prediction of the State of Charge is made, and until when the prediction is made. Balance Responsible Parties (BRPs) are required to submit their day-ahead portfolio at noon each day. Therefore, if a BRP wants to make a State of Charge prediction for the fleet of batteries they control, a BRP needs the prediction to be made in advance so that they still have time to determine the state of the total portfolio. This would also mean that the prediction for the State of Charge should cover the entirety of the coming day in order to be useful for the day-ahead portfolio.

Another aspect that is important to obtain from the models is the expected prediction error. Since the battery models have an inaccuracy range for low and high State of Charge, it is possible to solve this prediction error by trading energy. If a prediction error is expected, a solution would be to either buy or sell a certain volume of energy, to make sure the batteries stay in the range of accurate prediction. This puts the role of the accuracy of the prediction in the center of the energy trading strategy. Energy trading companies already heavily rely on their prediction mechanisms for energy generation and load profiles. This approach would remove the need to move around energy over the fleet of batteries, as is done with the optimization algorithms. Instead this approach uses the energy market as a way to optimize the prediction accuracy for a BRP. The level of abstraction of the battery models is also suitable for this, since the models can be used to simulate multiple batteries within a neighbourhood, but they can also be used at a higher level. Depending on the level however, different constraints might apply to the model. On a higher scale, it becomes increasingly difficult to transport energy between storage systems since the volume increases, and grid congestion plays a role. There is no guarantee that a BRP is allowed to transport energy, in order to increase the accuracy of their own prediction. Especially on a more national level, the odds of having sufficient transport capacity are shrinking rapidly with the increasing levels of grid congestion.

6.4 Social Impact

With the expected increase in batteries, a different problem also arises for the BRPs. A customer and homeowner will first and foremost want to install a battery for their own benefit. Yet, their interest might not always align with those of their energy supplier. The energy supplier, as a BRP might want to control the batteries in such a way that their prediction accuracy is as high as possible. This rises the question what the control strategy should be for batteries. A homeowner would want to make use of the energy is his battery for his own financial gain, yet this might impose temporary prediction inaccuracy if the battery becomes nearly fully charged or nearly empty. The energy supplier will have to make contractual arrangements with their customers, in order to optimally use the energy in the customers batteries. This most likely will results in a financial allowance per unit volume based on the energy prices paid by the BRP to the customer. However, this will further complicate energy contracts for customers, since a new component of energy pricing is introduced.

From this research, the question also arises who in the end is the party that carries the responsibility for the prediction error. If energy has to be traded in order to make up for the prediction error, this will most likely be done on the intra-day market. Prices on this market can be quite high, which makes it difficult to provide upfront transparency in permanent energy contracts. A solution for this would be offering dynamic pricing for customers, a strategy that is already being followed by several private energy companies in the Netherlands. This way, energy companies can delay applying pricing, until the moment of delivery. This way, there is a way to prevent inflexible contracts with set prices per unit volume.

Furthermore, if batteries are to become a staple in the energy transition, it is vital to take a look at the origin of intricate materials needed to manufacture batteries. Lithium is often sourced from brines and ores in Australia, Argentina, Chile, and China [41]. Some of these countries are known for having poor working conditions, and the mining business also is known to be high-risk for the miners. Therefore, in the scope of corporate social responsibility, it is wise to consider the impact of becoming reliant on materials whose extraction might negatively impact social responsibility in non-first world countries. Since lithium is not very stable as a metal, it is often found bound to other elements, which means that extensive treatments are necessary to produce lithium of quality high enough to use in energy storage. These processes are often energy and chemical intensive [42].

A point that will become important in the future is the end-of-life cycle situation with batteries. Since batteries have a limited lifetime of a finite amount of (dis)charge cycles, the disposal of batteries on a large scale can lead to problems. Batteries often contain chemicals that are harmful to the environment when released, as to which large-scale deployment of batteries calls for a well though through process for replacing, reuse, and recycling of batteries. Recovery methods are currently being developed and improved in order to extract lithium from batteries in the end-of-life phase, and to even do so in a sustainable way [43].

Chapter 7

Conclusion and Future Work

In this chapter, the results and discussion are combined in order to draw conclusions and to find answers on the research questions. The chapter will conclude with an outlook on possible future work that can be done based on this research.

7.1 Conclusions

From the results presented in this thesis, it is possible to answer the main research question such as posed in Chapter 2. However before this main question is answered, first, the different sub questions will be touched upon and answered individually. After this, the combination of answers on the sub-questions can be used to formulate a complete answer on the main research question.

What different modelling technologies are available?

From Chapter 3, it has become clear that many ways of digitally representing batteries have been developed over the last decades. However, for the application of State of Charge prediction, not all possible models are suitable. Models range from simple but inaccurate, to very complex requiring large amounts of information. Depending on the application and goals of the model, one might choose one model over the other. In this research, three models have been chosen for comparison; the Kinetic Battery model (KiBaM) by Manwell and McGowan [19], the Electrical Equivalent Circuit model (ECM) [10], and the Diffusion Buffer model (DiBu) by Homan [26]. Models that have been validated but have been left out of this research are the Diffusion model by Rakhmatov [22], the stochastic models such as by Chasserini and Rao [30], and the complex Dualfoil model by Doyle, Fuller and Newman [9].

How can the decision for a suitable modelling technology be made?

Depending on the technology of each battery, some models might be more suited than others. For batteries that show significant voltage recovery effects, the voltage prediction step of the Diffusion Buffer model is highly beneficial, since the State of Charge prediction is based on the voltage prediction in the model. However, if one is able to make measurements on the voltage behaviour of the battery, which would go at the expense of lifetime, one is able to use the ECM model, which behaves mode accurately. If one is unable to have any information on the voltage of the battery, which is not often the case, the KiBaM model provides a way out, since this model does not require a voltage prediction step in order to come relatively close to the actual battery behaviour. Next to this, a specific battery model can be chosen over others depending on the available information from battery suppliers, or on available measurement setups.

How can the battery model be applied to a fleet of batteries?

Every one of the three models applied in this work has its drawbacks. This drawback results in a prediction inaccuracy, which will have to be compensated for when making State of Charge predictions for fleets of batteries. Depending on the situation of the inaccuracy, this compensation can be done in multiple ways. Re-calibrating by means of measurement, trading energy, and smart control are some examples of workable solutions. If the prediction is made over a large fleet of batteries, one might opt for a model that does not require a voltage prediction step, like the KiBaM model. The introduced sum of voltage inaccuracies can lead to a significant deviation in prediction accuracy for the other models, as demonstrated by the original implementation of the diffusion buffer model. From this, it can be noticed that for a fleet of batteries, minimizing prediction errors is important, since prediction errors can sum up to significant deviations in energy volumes. Therefore, when applying a model that requires a voltage prediction step, it is desired to operate in the linear voltage region of the batteries, for which the optimization algorithms could be used as means. These algorithms calculate the optimal energy distribution over the entire fleet of batteries, such that the prediction error due to nonlinear voltage operation is minimized. For this, two models were proposed, an equal splitting algorithm, and a minimal energy algorithm. Comparison of the algorithm performance showed that the minimal energy algorithm performed better, by optimizing in less iterations and by moving less total energy.

How can battery energy storage models be applied smartly in energy trading?

When looking at the use of battery models, it is important to look at the role of the beneficiary. When energy is traded closer to moment of delivery, the prices rise. Therefore, it would be better to delay the selling of energy to as late as possible in order to maximize profit per unit volume of energy traded. In contrast, one would want to buy energy as soon as possible when the prices are low. Therefore, having an accurate forecast is vital. By making an accurate State of Charge prediction, one can already anticipate on the expected amount of energy that is available for trading. Therefore, one wants to have a prediction model that is as accurate as possible. Depending on the requirements and possible technologies of the battery fleet, one can choose the model that would lead to the smallest prediction error. From the results of the models, it concluded that the prediction can be made accurately for a time-frame of 24 hours, as this would heavily depend on the model accuracy and parameters. The maximum prediction horizon of the prediction model can influence the choice of the model, since a model that can provide a good prediction for a longer time-frame, can be used to buy energy earlier if necessary and sell energy later. Closer to the point of delivery of the energy the prices rise, so buying energy early for a lower price and selling energy closer to moment of delivery for a higher price is beneficial in order to maximize profits.

Having answered all the sub-questions, it is now possible to answer the main research question:

How can a suitable modelling technology be chosen to model a battery energy storage system?

In this work, we provide an overview of different modelling technologies for State of Charge prediction of battery energy storage systems. By taking a look at the desired output of the model, as well as the available data, such as battery technology, battery parameters, and available measurement setup, it is possible to determine an accurate model based on the scale of the battery. If voltage information is available from the BMS, one can apply a model like the ECM, since this applies a simple Coulomb counting method to determine the State of Charge quite accurately. This would require doing measurements on the open cell voltage as well as measurements over (dis)charge cycles, in order to determine the relation between terminal voltage and State of Charge. One could bypass this by doing measurements directly on the terminal voltage of the battery, providing a relation between the State of Charge and terminal voltage. This would take a few cycles to determine, which would decrease battery lifetime. However, if the model also needs to make a prediction on the voltage due to lack of information on the voltage as function of state of charge, one might opt for implementing the DiBu Model, as this model is capable of doing a voltage prediction too. However, determining the battery parameters for this model is quite complex, especially when one is only able to do measurements over an entire battery pack. As shown in Chapter 5, the linear regression algorithms used to determine the battery parameters ended up being relatively inaccurate, which showed in the voltage prediction step. Especially the initial parameters determined for the diffusion buffer model resulted in a very aggressive voltage prediction, reducing accuracy of the state of charge prediction. If one is able to accurately determine the battery parameters, it is expected that the DiBu model would perform the most accurately. If there is no information on the voltage, and this is also not measured, or relevant information from the BMS is not acquirable, implementing the KiBaM model could provide a viable alternative. This model, that works with a two-tank principle, does not require a voltage prediction, and is also incapable of making one.

7.2 Future Work

The results presented in this work show that three of the proven models are useful in State of Charge prediction for batteries. However, still some questions remain unanswered in the research field, and therefore, additional research can certainly be done in order to create a broadened overview of knowledge on battery simulation models. This section will touch on several possibilities for future work.

7.2.1 Battery Technology

Research into battery technology and application of models to several battery chemistry combinations might provide an overview on the influence of battery chemistry on the application of battery models. In this work, only one battery technology was applied, since this was the only available measurement setup. It might very well be the case that the analysed battery models are suited more for other battery technologies. For instance, the KiBaM model was designed specifically for Lead-Acid batteries. There is no certainty that the inaccuracy of the applied Kinetic Battery model is due to inaccuracy of the battery parameters, or that the KiBaM model is simply less suitable to model Lithium batteries.

7.2.2 Parameter Determination

As shown in Chapter 5, the accuracy of all models hinges on the model parameters. In this work, the battery parameters were only analysed on the level of the entire battery pack. Since the found parameters proved quite inaccurate, more research is required into the suitable methods to determine battery parameters. One could look at doing measurements on cell level, and see whether or not doing measurements on cell level would improve the prediction accuracy. This also ties in with the proposed future work of the previous section, since the preferred level to determine battery parameters might differ also on battery technology, but also between each battery model. In this work for instance, the the parameters β and γ were set to zero, due to the minimal effects of the voltage recovery effects the KiWatt battery showed. The effects of the voltage recovery effects are different in other battery technologies, meaning that for different battery technologies, certain parameters might be more or less important that for the technology of the KiWatt battery (LiFePO₄).

7.2.3 Battery Optimization

Two of the presented models (ECM and DiBu) make use of a linear voltage prediction as the base of the State of Charge prediction. However, the relation between Voltage and State of Charge is not fully linear. For high and low State of Charge, batteries show nonlinear behaviour. Therefore, a linear voltage prediction becomes inherently inaccurate in these regions of operation. For this there are two solutions; either expand the voltage prediction model in order to cope with this nonlinear behaviour, or prevent operation in the nonlinear region. In this work, two simple optimization algorithms were proposed in order to incorporate the second solution into the battery models. However, these algorithms can still be improved and expanded. Moving around energy in order to prevent prediction errors is always a less preferred option than increasing the prediction model accuracy. Moving around energy between batteries induces other problems, such as possible negative contribution to grid congestion, and conversion and transport losses. Therefore, research can be done on this nonlinear behaviour, in order to improve the battery models for the nonlinear voltage region of operation of the battery.

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