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Development of Physics-Based Models of Lithium-ion Battery Energy Storage for Power System Techno-Economic Studies

Vykhodtsev, Anton

UNIVERSITY OF CALGARY

Development of Physics-Based Models of Lithium-ion Battery Energy Storage for Power System Techno-Economic Studies

by

Anton Vykhodtsev

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Abstract

The pathway to achieving a sustainable, low-carbon power system includes the widespread integration of energy storage to tackle intermittency of renewable energy sources and provide stability to the grid through various grid services. Among the wide range of stationary energy storage technologies available, the lithium-ion battery dominates the growth in installations throughout the world. Although lithium-ion battery energy storage systems are complex grid assets with nonlinear characteristics and lifespans that depend on operating conditions, the majority of economic assessments are conducted using a simple energy reservoir model that does not consider the physical processes occurring inside the lithium-ion battery storage. This thesis focuses on the development of physics-based models for lithium-ion battery energy storage in power system techno-economic studies. The aim of this work is to assist developers and investors in making better-informed decisions.

In this work, modelling approaches used to represent lithium-ion battery energy storage in power system operation and planning studies are reviewed. The role of advanced models in enhancing the accuracy of economic evaluations and producing feasible schedules for battery storage providing transmission-level services is discussed. More importantly, this work proposes three physics-based mixed-integer models for battery energy storage for use in power system operation research studies. The first model is based on the single particle model and replicates the nonlinear operational characteristics of the battery. This model can be used for short-term operation studies. The second proposed model combines the widely-used energy reservoir model with the physical description of solid electrolyte interphase formation as a degradation mechanism. This model has been tested for long-term studies in both energy and power grid applications. Finally, the third proposed model is a data-driven model that accurately reproduces the degradation processes and nonlinear performance of the lithium-ion cell. The model facilitates long-term assessment of battery energy storage and effectively tracks both capacity and power fade over time. The results obtained from all the models are validated using the digital twin, which is based on the single particle model.

Preface

This thesis primarily has the manuscript-based format.

Chapter 2 of this thesis contains materials that have been published as:

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Chapter 5 of this thesis contains materials that have never been published, but they have been submitted for publication.

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To the brave people of Ukraine.

Glory to Ukraine!

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All models are wrong, but some are useful.

- George Box

Chapter 1

Introduction

1.1 Background and Motivation

The transition towards a more sustainable global economy is impossible without a wide energy transition. One of the key elements of the energy transition is the integration of a relatively new asset class for power systems: lithium-ion battery energy storage system (LIBESS). Lithium-ion batteries have already demonstrated their usefulness and potential in achieving decarbonization of the power grid, enhancing its reliability, ensuring its stability, and bolstering its resilience within a remarkably short timeframe [1, 2]. As an example, the Kapolei Energy Storage project is set to be commissioned in 2023 in Hawaii [3]. This battery facility, with a capacity of 185 MW/565 MWh, will play a crucial role in load shifting and frequency regulation for the Hawaiian power grid. In conjunction with local solar and wind farms, it will serve as a replacement for the recently closed coal-fired plant, resulting in a significant reduction in greenhouse gas emissions. Moreover, during September 2022's record heat wave, the California Independent System Operator highlighted a specific factor that contributed to the reliability of the grid to meet peak demand: the presence of 3,500 MW of installed battery storage in the system [4]. An example of how batteries help to maintain grid stability comes from the National Grid in the United Kingdom. Currently, almost all of the firm frequency response services are procured from lithium-ion batteries [5]. This is a significant shift compared to 2014 when the contribution of batteries to this service was zero. The presence of LIBESS in Texas power grid proved to be important in enhancing resiliency during the extreme heat of June 2023. When a nuclear plant and a large coal facility unexpectedly tripped from the grid and failed to supply power, the grid operator was able to quickly dispatch batteries, ensuring an uninterrupted energy supply [6].

The implementations of LIBESS in the power grid discussed above are not sporadic examples; rather, there is a consistent trend of an increasing number of LIBESS installations worldwide. This trend can be attributed to various factors such as the improvements of technology [7], economy of scale [8], enhanced bankability [9], and new regulatory initiatives [10]. Annual additions to the total installed capacity worldwide grew from 0.3 GW in 2015 to 16 GW in 2022 [11, 12]. Although the USA's utility-scale battery storage is projected to more than double from April 2023 to April 2024, increasing from 10.4 GW to 20.3 GW [13], a new set of policies in China is set to establish China as the leading country in stationary battery energy storage by 2030, surpassing all others in terms of power capacity [14].

The emergence of grid-connected LIBESS is aligned with the overall potential of stationary energy storage for the grid. According to a study by the US Department of Energy on storage [15], energy storage can act as an important participant in the electricity market. It can provide services such as economic energy arbitrage, frequency regulation, and spinning reserves. In a power grid with a high penetration of solar and wind power generation, renewable energy time shifting is facilitated by energy storage. Additionally, it can be utilized for transmission upgrade deferral or relieving transmission congestion. Energy storage located behind-the-meter can be employed for managing demand charges and net metering.

Although there are other energy storage technologies available, such as pumped storage hydropower, compressed air energy storage, lead-acid batteries, redox flow batteries, sodium-based batteries, flywheels, hydrogen energy storage systems, and gravity energy storage, it is the lithium-ion battery energy storage that is leading the growth of the energy storage market [12]. There are several reasons for this trend. The pumped storage hydropower accounts for over 90% of the total global electricity storage in 2020 [12]. However, it has certain limitations. Firstly, it is geographically limited. Secondly, it requires a significant amount of time to construct. Additionally, obtaining the necessary permits for its installation can be challenging. Lastly, it is considered an expensive asset class. The compressed air energy storage and hydrogen energy storage system are less energy efficient when compared to LIBESS [16]. The lead-acid batteries have a shorter cycling life [16]. The credibility of redox flow batteries for investors, as well as the use cases for longer duration storage, are questionable. The flywheels have only one use case, which is for frequency-regulation services [15]. The construction of gravity energy storage is more complex compared to the installation of LIBESS. Molten sodium batteries have been available for a considerable period of time, but they have not found wide application due to their high temperature requirement. On the other hand, sodium-ion batteries are still in the early stages of development and commercialization.

However, when compared to other infrastructure elements of power systems, lithium-ion batteries prove to be a highly complex asset class. Apart from a sophisticated revenue stack that relies on a rigorous understanding of local regulatory frameworks and power market conditions, lithium-ion batteries present significant challenges as electrochemical systems. Their physical performance exhibits strong nonlinearity and deteriorates over time. To achieve a positive financial return, it is crucial for the owner of a LIBESS facility to combine trading analytics with an accurate description of the physical dynamics of the LIBESS, thus optimizing its overall performance.

1.2 Literature review and gap identification

The stationary LIBESS can be integrated into the electrical grid in multiple ways. It can function as a standalone merchant [17] or a grid service provider facility [18], be a part of the hybrid plant [19], serve as a transmission grid asset [20], or operate as a behind-the-meter facility [21]. Each of these applications has specific operating conditions [1]. Moreover, market regulations and market dynamics define the technical requirements for how the storage should operate. The impact of uncertainty from either renewable generation or the behavior of other market participants also affects the energy storage operation. All mentioned above influence the strategic operation and long-term planning of lithium-ion battery storage. From a mathematical point of view, the search for the strategic dispatch and LIBESS integration plan is usually formulated as mathematical programming. The key component of this optimization framework is a set of constraints or modifications to the objective function that correspond to the battery model.

1.2.1 Gap identification 1

There are plenty of review papers that discuss and summarize the integration of energy storage into the grid, as well as its associated optimization problems, from technical and mathematical perspectives. A well-structured summary and classification of optimization frameworks and market models for stationary energy storage used in operation and planning problems at the transmission and distribution levels were developed by Miletic *et al.* [22]. Although a standard energy reservoir model and some of its modifications were discussed, more detailed LIBESS models and their significance for operation and planning studies involving various LIBESS applications with different LIBESS application were beyond the scope of the paper. A detailed review of the lithium-ion battery storage for the power grid applications with focus on the relationship between the lithium-ion cell technology and the LIBESS short-term and long-term operation, the architecture and topology of LIBESS, and grid services was conducted by Hesse [1]. Additionally, available simulation tools to evaluate LIBESS performance were also discussed. While optimization frameworks for storage control and placement were discussed, methods for representing lithium-ion batteries within these frameworks were not discussed. Various optimization methodologies, variety of decision-making horizons, ways to tackle uncertainty, and solution techniques were summarized by Weitzel [23] as a part of the review of energy management systems for stationary energy storage. However, only a generic Power-Energy Model with several empirical aging degradation assessment methods were part of the discussion. The critical review of three models of LIBESS, namely the energy reservoir model, the equivalent circuit model, and the electrochemical model, was provided to the power system research community by Rosewater *et al.* [24], where they used them to calculate the optimal schedule of a LIBESS for a peak shaving application. The authors outlined the advantages and disadvantages of each model from a computational point of view but they mostly reviewed references outside of typical system-level grid applications of LIBESS. The authors of [25] limited their review to the transmission congestion relief application of stationary batteries. They focused specifically on regulation, project costs, and evaluation metrics. The consideration of battery modeling was done in relation to available commercial tools for determining the value of the project. The benefits of using stationary energy storage for the electrical grid and an overview of energy storage technologies are presented in [26] and [16]. However, the approach to battery modeling was not discussed. The architecture of energy storage, grid energy storage applications, the role of the energy management system, and optimization frameworks were addressed in [27]. Several review papers, such as [28] and [29], have focused on lithium-ion battery modeling and state variable estimation in general, without specifically addressing LIBESS models suitable for use in operational research.

In summary, a gap was found in the literature regarding the overview of LIBESS models used in techno-economic analysis of power systems in the context of LIBESS grid applications.

1.2.2 Gap identification 2

The lithium-ion battery energy storage is usually formulated in power systems techno-economic decision-making studies using a simple linear energy reservoir model [30]. This model does not account for the system's high nonlinearity, which can result in the battery operating outside the safety range when providing committed grid services. Moreover, relying on a simple battery model leads to overestimation of revenue in a techno-economic assessment [31].

Researchers have proposed several models in the literature to incorporate the description of the physical system behind LIBESS and enhance its short-term performance in the optimization framework environment. Sakti *et al.* [31] developed a mixed-integer linear battery model that incorporates the energy efficiency as a function of the charge and discharge power, as well as the state of charge. When using the energy arbitrage application for the storage facility as a case study, the dispatch obtained with a simple energy reservoir model with constant parameters overestimated revenue by 10% compared to the proposed model. Although their model was built from first principles, it was empirical in its formulation. Only the discharging characteristics were used to estimate parameters of the model for both charging and discharging performance, which is not valid according to [32]. The authors of [33] studied the optimal operation of LIBESS deployed in the IEEE-14 system to profit from economic energy arbitrage. Their LIBESS model was based on a simple linear energy reservoir model, where fixed parameters were substituted with ones dependent on the state-of-energy. The justification for employing a non-linear dependence between energy efficiency, charge/discharge power, and state-of-energy was based on the empirically constructed equivalent circuit model based on the underlying physical phenomena from [34]. In [32], the energy reservoir model was enhanced by incorporating the dependency of charging power on the battery state of energy. As a result, the strategic dispatch using this model achieved a 20% increase in revenue compared to the observed dispatch based on a simple model. Experimental verification confirmed that the calculated dispatch with the simple model was unable to deliver the committed energy. The optimal bidding strategy in the frequency regulation market for the electric vehicle aggregator, considering different participation scenarios, was outlined in Vagropoulos' study [35]. Their model successfully simulated the transition from constant current mode to constant voltage mode of charging operation by incorporating a functional dependence on the state of energy. The authors reported a cost reduction difference of 19.5% compared to a simple model. Taylor *et al.* [36] utilized a linearized equivalent circuit model of LIBESS to derive the optimal schedule for peak load shaving. They estimated the parameters by analyzing cycling data obtained from their experiments with Lithium iron phosphate cells. A more accurate model significantly reduces the mismatch between the optimized schedule and the same schedule corrected by the battery management system in the test. The model, in terms of decision variables of the equivalent circuit model of a lithium-ion cell (voltage and current), is formulated and integrated into the nonlinear optimization framework in [19]. Here, the dispatch for PV generation smoothing, derived with the proposed model, avoids unsafe operation compared to a dispatch obtained with a simple energy reservoir model. Nguyen *et al.* [37] constructed their nonlinear battery model using the equivalent circuit model and tested it within the optimization framework to find the strategic operation of LIBESS in the energy and reserve markets using the forward dynamic programming algorithm. Although their approach did not guarantee global solution to the optimization, their model was able to identify operating range of the battery with higher energy efficiency. In [24], the energy reservoir model, the equivalent circuit model, and the electrochemical model were used in nonlinear optimization problems for a peak shaving application. However, the authors did not address the difference in calculated dispatches between each model and whether scheduling with a less advanced model leads to the operation outside of the safe operational range. The physics-based model, specifically the single particle model, was utilized in two separate studies: Reniers [38] for deriving scheduling of LIBESS in the energy market, and Cao [39] for deriving scheduling of LIBESS in the frequency regulation market. Both authors constructed a nonlinear optimization problem and focused on the impact of degradation. However, they did not assess the nonlinear system dynamics of their proposed model and no comparison was performed with a simple linear reservoir model in this regard.

Overall, short-term operation models of LIBESS for use in power systems optimization studies can be categorized into two types: empirically built models with various assumptions (as discussed in [19,31–33,36,37]), and models built from first principles that result in a non-linear optimization framework (as described in [24,38,39]). The literature lacks physics-based short-term operation LIBESS models that can be integrated into mixed-integer optimization problems of the power system.

1.2.3 Gap identification 3

Lithium-ion battery energy storage is a reliable alternative to conventional generation. However, besides the significant capital cost, the battery's long-term performance deteriorates over time due to calendar aging and with the number of charging/discharging cycles, known as cycle aging [40]. Therefore, it is crucial to include a degradation description that occurs in the battery when looking for planning and operational decisions with LIBESS. The mathematical formulation of degradation for lithium-ion battery energy storage, used in techno-economic studies for power systems, can be classified into three broad categories: established empirical models that rely on information from the manufacturer's datasheet or experimental observations, custom non-linear empirical models, and physics-based models. All these degradation approaches can be integrated into the optimization as a set of constraints or as the cost of degradation in the objective function.

The established empirical models are mostly focused on cycling ageing and are categorized into state of energy/ state of charge (SoE/SoC) restrictions as constraints [17, 41], the energy throughput method [17], the Rainflow or cycle-counting algorithm [42]. The box constraints on SoE/SoC as part of the battery model were suggested in [17] and [41]. Although restricting the SoE range of the battery can decrease short-term revenue, it has been shown that employing the battery for energy arbitrage, providing reserves, and frequency regulation within the optimal SoE range [41] can 100% increase the expected lifespan of the battery and, as a result, generate more long-term revenue. A similar methodology to limit

SoE was used for the energy arbitrage application in [17] and for peak shaving and frequency regulation in [43]. Overall, the degradation model based on SoE/SoC restrictions is useful to avoid overcharging and overdischarging. However, it lacks important factors influencing aging, such as cycle depth, current rate, and average SoC. Additionally, it does not assign a price for degradation to discourage cycles with lower revenue. According to the energy throughput concept, a lithium-ion battery is only capable of charging and discharging a finite amount of energy over its lifetime. This means that capacity loss is proportional to the amount of energy cycled through the battery over the given operation horizon. The optimization framework can integrate the energy throughput method either through the degradation replacement cost [17] or enforcing limits on the number of full charging/discharging cycles performed daily [44] or annually [45]. Although the energy throughput method is an attempt to include the common warranty provided by a LIBESS manufacturer and is a suitable way to include the cost of degradation in optimization, the method does not consider the nonlinear complexity of lithium-ion battery aging mechanisms. The Rainflow algorithm assumes that shallow discharge cycles degrade lithium-ion batteries less compared to deep discharge cycles [42]. Although, the Rainflow algorithm is nonlinear by its nature and it cannot be formulated in closed form, several methods have been proposed in the literature. A piecewise linear approximation method was introduced by Xu *et al.* [42]. The linearization of the long-term model with the Rainflow algorithm was performed using Benders' decomposition in a study on battery storage in energy and regulation markets by Kazemi [46]. A nonlinear optimization with the Rainflow algorithm was constructed to find strategic scheduling of LIBESS providing peak shaving and participating in energy trading [47]. In contrast to the energy throughput concept, the Rainflow algorithm captures some nonlinearities; however, it still does not include factors such as current rate or average SoC. Moreover, the discussed above models are only focused on cycling aging.

In the literature, custom-built empirical models have been introduced to overcome the limitations of the Rainflow algorithm and the energy throughput method. Maheshwari *et* *al.* [48] developed an empirical degradation model, incorporating dependencies on charging/discharging current and SoE, to address these limitations. They applied this model to the energy arbitrage application scheduling of LIBESS and also demonstrated the inaccuracies in degradation estimates obtained through the energy throughput method. The strategic dispatch for LIBESS in the energy and reserve markets was derived in [49] using a degradation cost function based on the depth of discharge (DoD), discharging rate, and a mixed-integer linear optimization framework. Hesse *et al.* [50] derived the strategic operation of LIBESS in the electricity arbitrage application by utilizing a degradation model that is based on the energy throughput and the dependency of the energy capacity fade on the charging power. They incorporated this model into their mixed-integer linear programming, which was solved for a one-month operation period. The SoE-dependent degradation model was explored and compared with the Rainflow algorithm and the energy throughput method for energy arbitrage in [51]. The utilization of this model yielded the optimal balance between market revenue and degradation levels. The linearized nonlinear degradation models described above share a common drawback: they distinguish between degradation contributions from SoC, DoD, and charging/discharging current but do not include calendar ageing. However, the ageing described by these models results from one dominant degradation process, namely the growth of the solid electrolyte interphase (SEI) formation [52]. Additionally, the utilization of linearization techniques in these models leads to an increase in computational time.

The physics-based models depict the underlying physical system of the lithium-ion battery. Reniers [38] and Cao [39] incorporated the physics-based model, specifically the single particle model, along with a mathematical formulation of SEI growth, as a main degradation process to obtain strategic dispatch of LIBESS participating in electricity arbitrage and providing frequency regulation services, respectively. The use of this model within the optimization framework leads to a non-linear optimization problem. The optimality of the solution for this problem is not guaranteed. It is difficult to solve this problem without the right initial guess, and convergence can be a challenge, often requiring a significant amount of time to achieve a solution.

Overall, the literature indicates the existence of two distinct groups of LIBESS models with degradation for optimization studies. One group consists of simple linear models that are built upon limited observations, while the other smaller group comprises nonlinear models constructed based on physical laws. However, in the existing body of research, there is no simple linear model available that incorporates a physical description of degradation.

1.2.4 Gap identification 4

The mathematical model of a lithium-ion battery is required for the correct functioning of the battery management system. Using this model the battery management system is be able to estimate various internal states of the battery, such as SoC or state of health (SoH), which cannot be directly measured. The monitoring of safety operation to avoid over-charging and over-discharging is also conducted by BMS using the mathematical model of lithium-ion cell. In recent years, alongside conventional physics-based electrochemical models and electrical equivalent circuit models, data-driven models have also gained popularity in lithium-ion cell community [28]. The literature provides a wide selection of data-driven methods to estimate SOC/SoE an SoH such as feedforward neural network [53,54], extreme learning machine [55], support vector machine [56], nonlinear autoregressive neural network [57], Gaussian process algorithm [58], wavelet neural network [59], and self-supervised transformer model [60], and physics-informed neural network [61].

The list of these data-driven approaches for battery simulation is not limited to the methods mentioned above. However, there is a limited number of papers where data-driven models have been integrated into the optimization framework to derive strategic scheduling of LIBESS. Zhao *et al.* [62] constructed a neural network to predict degradation by incorporating aging factors such as ambient temperature, charging/discharging rate, SOC, DOD, and current SOH as inputs. The dispatch of LIBESS, placed in a small microgrid with renewable generation plants, was performed iteratively using a standard optimization framework. The framework was updated in each iteration with results obtained from the knowledge generated by the neural network. This approach heuristically decouples optimization from degradation assessment, which means it cannot guarantee the optimal operation of LIBESS and the efficiency of obtained solution. In the study by Cao [63], a deep reinforcement learning method incorporating operation-dependent energy efficiency based on the equivalent circuit model and a linearized approximation of the Rainflow algorithm for degradation assessment was employed for LIBESS participating in the energy arbitrage. The utilization of a model-free approach yielded more accurate revenue estimates in comparison to the traditional model-based optimization method. Kwon *et al.* [64] utilized reinforcement learning algorithm to derive operational policy for LIBESS owner providing energy arbitrage and frequency regulation services simultaneously. Nonlinear cycle-based battery degradation based on the Rainflow algorithm was used in their model that demonstrated superior performance compared to the linearized degradation model proposed in [63]. In [65], an extreme learning machine was used to model and incorporate the degradation of LIBESS in the vehicle-to-grid demand peak shaving operation problem. The degradation model, trained using data generated from empirical DoD and charging/discharging rate stress functions, was introduced into the optimization framework. The advantage of the extreme learning machine lies in its inherent linearity, as it lacks activation functions in its architecture. Overall, the LIBESS aging model they developed yielded an energy capacity loss comparable to that estimated by the Rainflow algorithm, while requiring less computation time.

Although various data-driven models for LIBESS in power system optimization studies have been proposed, they were all constructed based on empirical approaches. These models did not take into account the actual energy and capacity fade in their constraints and lacked consideration for the short-term performance of LIBESS. Moreover, these models were either heuristically designed [62], unconventional in the field of operations research [63, 64], or only applicable for linear assumptions [65].

1.3 Thesis objectives

The overall objective of this dissertation is to propose new physics-based lithium-ion battery models for use in power system techno-economic analysis. This is a timely and relevant research direction as the deployment of LIBESS increases every year throughout the world, and the most common practice nowadays is to use a simple linear model, such as an energy reservoir model, for the assessment of these projects. While the primary focus of this work is lithium-ion battery energy storage, the proposed methodology is applicable to other battery technologies based on porous electrode theory. This research is expected to help modellers and decision-makers in power system studies obtain more accurate estimates of the benefits of installing LIBESS, as well as maintain the safe operation of the battery. The specific objectives that correspond to identified gaps are listed as follows:

1. To provide a comprehensive overview of publications on the techno-economic analysis of grid-connected LIBESS in power systems, with a specific focus on the battery models employed in optimization frameworks used in these papers. The aim is to emphasize the significance of utilizing advanced modeling techniques and their impact on the decision-making process. This will assist modelers in selecting an appropriate battery model that aligns with their requirements for energy management in LIBESS. Furthermore, potential directions for future research, exploring/using the utilization of detailed battery models in techno-economic studies of power systems, are also discussed.

2. To propose a linearized physics-based model of a lithium-ion battery for short-term operation, suitable for integration into a mixed-integer optimization framework for power system operation research studies. This model should accurately describe the physics of the processes occurring inside the battery while remaining computationally efficient. Consequently, it will maintain the nonlinear functional relationship between allowable charging/discharging power, SoC, and energy efficiency. In addition, the proposed model should be compared with the widely used energy-reservoir model. The study should demonstrate that the proposed model generates feasible strategic dispatch and provides accurate economic assessments, in contrast to a simple energy-reservoir model.

3. To enhance the representation of battery degradation in power system economic assessment, it is crucial to develop a physics-aware degradation model of lithium-ion battery system. This approach should be computationally efficient while effectively capturing battery degradation. Moreover, the model should be readily integrated into the mixed-integer linear programming formulation. The model should have a hybrid structure combining linearity of the energy reservoir model and complexity of the physics-based ageing description. Additionally, a digital twin should be created to validate the results obtained with the proposed model. This digital twin would utilize an actual electrochemical model, single particle model, of the lithium-ion cell with degradation caused by SEI growth.

4. To develop a data-driven, physics-based model of a lithium-ion battery energy storage system that accurately replicates the nonlinearity of both performance and degradation processes under varying operating conditions. This AI-assisted model should be constructed in a manner that enables its integration into traditional mathematical optimization frameworks. The proposed model should undergo long-term performance testing to evaluate its credibility for the typical LIBESS application.

1.4 Thesis structure and contributions

The rest of this thesis is organized as follows. In Chapter 2, various modelling approaches to lithium-ion batteries for operation research tasks in power systems studies are reviewed. The focus is on grid-connected LIBESS at the transmission level. The principles and mathematical formulations of three main types of battery models that are used to derive optimal scheduling for different energy storage applications are discussed. These models include descriptions of battery short-term operation and degradation. Additionally, the features and types of the corresponding optimization frameworks are summarized. The impact of using a more detailed battery model on the economic benefits and feasibility of dispatch for LIBESS applications such as economic energy arbitrage, frequency regulation, operating reserve, demand peak shaving, renewable integration assistance, and transmission upgrade deferral is examined. Finally, a survey of the reviewed studies with respect to findings is conducted.

Chapter 3 introduces a novel physics-based model for a lithium-ion battery. This model is specifically designed to be used within the mixed-integer optimization framework to derive short-term strategic operation of LIBESS providing various grid services. The basis for this model is the single particle model of the lithium-ion cell. Additionally, the chapter discusses the techniques employed for linearization and the assumptions made during the model's development. To evaluate the effectiveness of the proposed model, it is tested in energy arbitrage strategic operation. The results obtained from this case study are then compared to those obtained using the traditional energy-reservoir model. The proposed physics-based model successfully captures the nonlinear operational characteristics of the battery. To verify the feasibility of the strategic scheduling, a digital twin is constructed based on the original single particle model.

In Chapter 4, a hybrid physics-aware lithium-ion battery model, which is based on the energy-reservoir model and incorporates the physics of the SEI formation as an aging mechanism, is proposed. This model is constructed as a mixed-integer linear model and assumes that the voltage of the lithium-ion cell remains equal to the nominal voltage of the cell under all operating conditions. By adopting this approach, the proposed battery model can be integrated into mixed-integer optimization frameworks, offering a significant advantage, such as providing an accurate physics-based estimate of degradation. The proposed model is evaluated using both power- and energy-based use cases from the electrical grid. Furthermore, the performance of the proposed model is compared to other degradation models, such as the energy throughput method and the Rainflow algorithm.

Chapter 5 introduces an AI-assisted model for a LIBESS, which accurately replicates the degradation processes and nonlinear performance of the lithium-ion cell. This model consists of three neural networks that have been trained using datasets derived from the actual physics-based lithium-ion cell model. The proposed neural network architecture enables its integration into mixed-integer optimization frameworks. This model is used for both long-term and short-term energy arbitrage studies. The model tracks both capacity and power fade. The model is validated using the digital twin and compared with the widely-used energy reservoir model with the energy throughput method for formulation of degradation.

Finally, in Chapter 6, the concluding remarks and suggestions for future works are provided.

Chapter 2

Modelling Approaches to Characterize Lithium-ion Battery Energy Storage Systems in Techno-Economic Analyses of Power Systems[1]

2.1 Introduction

The number of lithium-ion battery energy storage systems (LIBESS) projects in operation, under construction, and in the planning stage grows steadily around the world due to the improvements of technology [7], economy of scale [8], bankability [9], and new regulatory initiatives [10]. It is projected that by 2040 there will be about 1,095GW/2,850GWh of stationary energy storage in operation mostly in the forms of batteries [66]. In particular, grid-connected LIBESS deployments are expected to grow significantly from 1.5 GW in 2020 to 8.5 GW in 2030 [67]. The emergence of the grid-connected LIBESS is also in line with the potential for the grid from a stationary energy storage in general [16, 25, 68].

LIBESS projects for grid applications require high capital cost, compared with conventional solutions, encounter deteriorating battery characteristics as they age, and face revenue risks associated with continuously changing regulatory and electricity market policies. Nevertheless, their economic performance is mostly simulated and assessed using simplistic black-box representations of battery operations [69] along with an empirical relationship to characterize ageing [70]. Particularly, strategic operation of LIBESS to maximize revenues or the corresponding optimal sizing and placement decisions associated with LIBESS are defined through optimization models. Such models often include constraints associated with market opportunities and the short- and long-term operation of LIBESS. The former depends on the particular application whereas the latter in intended to duplicate the physical performance of LIBESS. However, under the "black-box" paradigm, LIBESS are treated as a reservoir of electrical energy with a nominal efficiency. In this work, this model is also referred to as the Power-Energy Model. The given model does not take into account the actual chemical processes inside the battery pack and how they impact the battery operation. The main advantage of this approach to LIBESS modelling is its simplicity and the reduced computational complexity of large-scale optimization models. However, a growing evidence points that the short-term operation and long-term planning of LIBESS projects would likely benefit from detailed models of LIBESS [32, 71] that go beyond a simple Power-Energy Model. For example, a lithium-ion battery storage is often used to provide multiple energy and ancillary services for the electrical grid to enhance asset utilization and economic benefits to the owner [72]; in such cases, the optimal market participation calculated using a simplistic Power-Energy Model may lead to the execution of infeasible operations and an erroneous estimate of economic costs and revenues [36]. This occurs because a simple Power-Energy Model does not accurately reflect the dynamics of chemical processes inside a lithium-ion cell, which is the main component of LIBESS. This can be more pronounced if the operation and planning of LIBESS for power systems is performed over multi-scale time horizons. In particular, control strategies for participating in energy and ancillary services markets encompasses alternative time scales (e.g., hours for energy, minutes for operating reserves and seconds for frequency regulation). The linkage of these timescales will likely be inaccurate if a simple black-box model is used. This is because the battery is often simulated using one single time scale, usually in hourly intervals, based on its power output, usually in MW. Degradation, however, occurs continuously and accumulates over years [73]. The data from a few available experimental research works also supports the importance of considering more detailed models for operation [32, 36] as well as for the long-term performance [38] of batteries.

In a pioneering work published in 1985, the techno-economic assessment of battery storage application was performed by Sobieski [74] where the author compared battery energy storage with combustion turbines for peak shaving capacity expansion and for spinning reserve. Over the years since, the strategic battery operation in various decision-making studies in power systems have been modelled using generic models without a reference to a particular battery technology. Miletic and co-workers [22] summarized and structured optimization frameworks and market models for stationary energy storage used in operation and planning problems on the transmission and distribution levels. A standard Power-Energy Model and some modifications were discussed as well. However, the impact of including additional details into the simple battery model was not assessed. Recently Hesse *et al.* [1] conducted a detailed review of the lithium-ion battery storage for the power grid applications where the relationship between the lithium-ion cell technology and the LIBESS short-term and long-term operation, the architecture and topology of LIBESS, and provided services to the grid were discussed. In addition, the simulation tools for stationary battery were presented and their characteristics were classified. However, the optimization frameworks were only mentioned briefly, and the approaches to the lithium-ion battery representation in these frameworks were not discussed. The comprehensive review performed by Weitzel [23] provides valuable insight into the energy management systems for the stationary energy storage in general. The authors classified optimization techniques, scopes of the model, decision-making horizons, uncertainty formulation, and solution methodology with respect to different studies with the stationary storage. Despite the fact that a generic Power-Energy Model was discussed and several empirical ageing models were examined, the study did not focus on modelling of LIBESS in operation and planning techno-economic studies.

The lithium-ion battery community suggests a variety of models with different levels of accuracy and computational complexity for simulation [75] and characterization of ageing [52]. These models are usually employed in the battery management system (BMS) to predict battery behaviour and to estimate state-of-charge or state-of-health of the battery [27]. Until recently the strategic operation of stationary LIBESS was derived using advanced battery models by only a few researchers [38, 39]. The critical review of three models of LIBESS, namely the energy reservoir model (referred to as the Power-Energy Model in this study), the charge reservoir model (referred to as the Voltage-Current Model in this study), and the concentration-based model (referred to as the Concentration-Current Model in this study), were provided to the power system research community by Rosewater *et al.* [24] where they used them to calculate the optimal schedule of a LIBESS for a peak shaving application. The authors outlined the advantages and disadvantages of each model from a computational point of view but they mostly reviewed references outside of typical system-level grid applications of LIBESS.

The contribution of the present review paper is to provide a detailed overview of alternative lithium-ion battery models and how they have been used to represent grid-connected LIBESS at the transmission level in electrical power system studies. This will help modellers to select an appropriate battery model that fits their needs in the energy management of LIBESS. The data collected from the surveyed papers can be utilized for constructing appropriate optimization frameworks. In particular, we focus on papers that have integrated transmission-connected LIBESS into grid operation and planning techno-economic studies. This paper builds on previous works; for example, it extends the work presented in [24] where the models were presented but no discussions of their application in techno-economic optimization problems were conducted. Compared with [22], where different optimization models for energy storage operation and planning were summarized, and with [27], where optimization protocols and frameworks for LIBESS applications were addressed, in this review paper, various applications were examined from the perspective of how the lithium-ion battery was described and represented. The review work [76] was focused on the battery models for the BMS and the architecture of LIBESS and BMS. Their case study only addressed optimal charging scheduling for the combined LIBESS-photovoltaic generation plant considering physics-based model whereas in this paper a broader range of LIBESS applications is examined. Compared with [23] the novelty of our study includes mapping the lithium-ion battery models to the optimization frameworks utilized in operation and planning studies for power systems. The review of [1] is in line with the LIBESS application scope of our paper but it does not study the impact of battery models on the evaluation of the LIBESS projects. There are numerous studies at the power distribution level [22]; those papers often use a simple Power-Energy Model and are not included in this review.

The remainder of this paper is structured as follows: the next section gives an overview of LIBESS models, the third section presents examples of economic studies with LIBESS providing different services, the fourth section discusses and summarizes the impact of LIBESS models on the strategic operation and planning.The outlook on future research and concluding remarks are also given there.

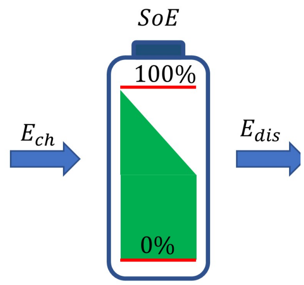
2.2 An overview of the lithium-ion battery modelling approaches

A battery is an electrochemical device that is able to store electrical energy in the form of chemical energy and to convert it back to electrical energy when it is needed. Since their invention in 1800 by Alessandro Volta, various battery technologies have emerged;

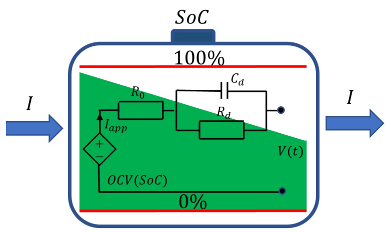
however, in this work, we are focused on the lithium-ion technology. This type of battery was pioneered by Whittingham [77], significantly improved by Goodenough [78], and brought to the market by Sony in early the 1990s. Today, the term battery is often used to refer to the electrochemical storage as a whole system. In fact, each battery consists of a pack of elementary electrochemical units – cells. The way the cells are connected in the battery (in parallel and in series) determines the battery's nameplate ratings. A cell is a physical place where the conversion occurs and where the electrochemical energy is stored.

The battery models by the extent of description of the physical processes and corresponding safety constraints can be divided into black-box, phenomenological, and physical models [79, 80]. In the black-box model or the Power-Energy Model as it is referred in this paper (Fig. 2.1a), a battery is replaced with a reservoir or a bucket, where energy comes in and comes out. This model does not consider a description of the physical phenomena inside the cell. If the phenomenological model or the Voltage-Current Model as it is referred in this paper is used (Fig. 2.1b), the battery is replaced with the system that was empirically built to replicate the response of the battery to the control commands [75]. The electrochemical process inside the battery and the response of the cell to external factors are accurately described using the physical model or the Concentration-Current Model as it is referred in this paper (Fig. 2.1c) [79].

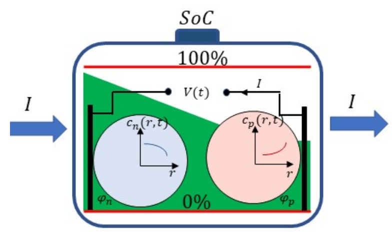
The long-term performance of the lithium-ion battery deteriorates with time (calendar ageing) and with the number of charging/discharging cycles (cycle ageing). There are several mechanical and electrochemical processes that gradually deteriorate either energy capacity, rated charging/discharging power, or both. The ageing of the lithium-ion cells is impacted by environmental conditions, such as high and low temperatures, operating conditions, such as high charging/discharging current and high/low state-of-charge, and even when the battery is at rest [81]. The degradation of the lithium-ion cell is usually accompanied by loss of lithium inventory or loss of active material of an electrode. The lithium inventory is consumed by various side reactions. The decline of the number of cyclable lithium leads to



(a) Power-Energy Model



(b) Voltage-Current Model



(c) Concentration-Current Model

Figure 2.1: The lithium-ion battery models used in techno-economic analysis of power systems.

a decrease in energy capacity and by-products of these parasitic reactions create additional internal resistance of the cell that reduces the available charging/discharging power capacity. Examples of such processes are solid electrolyte interphase (SEI) film growth and lithium plating. The SEI formation is considered as a dominant degradation mechanism [52]. The SEI is mostly formed on the surface of the negative electrode during charging since these conditions favour electrochemical decomposition of electrolyte [82]. The lithium ions can also be converted to metallic lithium which is deposited on the electrode through the lithium plating process. The structural changes, such as cracks in the electrode particles or dissolution of material in electrolyte, lead to loss of electrode active material. More detailed information on the degradation mechanisms in the lithium-ion cell can be found in [81], [83], and [52].

In power systems techno-economic studies literature, the battery is often modelled from two extreme viewpoints: the system level and the the cell level. The system level method presents only high-level description of LIBESS and treat it as a single unit that can store and supply energy following the instructions from the operator. The narrative of the second method is only focused on the precise characterization of the operation of one lithium-ion cell. Only these methods will be discussed in this paper. In reality, actual LIBESS includes a set of lithium-ion cells, the energy conversion system, the battery management system, and the thermal management system [84]. The impact of the thermal and conversion systems on the decision-making process is mostly out of consideration in these papers since only few researchers added them to the battery model [17, 19, 24, 50].

In this section, the battery models that can be found in power system operation and planning papers are reviewed. These models encompass both operation and degradation descriptions. The model for the battery operation is coupled with corresponding model for ageing that uses the same state variables. The ageing description formulations are limited to the ones found in the techno-economic analysis of power systems.

2.2.1 Power-Energy Model

The simplest model of the battery assumes that the battery can be seen as an energy reservoir in which the energy is pumped to store and from which the energy is drawn to consume (Fig. 2.1a). If such a model is used for analysis there is no need to distinguish elementary electrochemical units or the type of electrochemistry within the battery. This is the most popular model to characterize the operation of the battery in techno-economic studies in power systems. It is likely that this modelling approach has come from the mature pumped hydro energy storage modelling that was around for a long time [85]. The control variables for this model are charging, ch_t, and discharging, dis_t powers whereas state-of-energy, SoE_t, is the only state variable. The state-of-energy indicates the present value of energy (often in MWh in power systems literature) stored in the battery. The LIBESS is not an ideal system, thus there will be losses during the charging/discharging cycling. The loss in a Power-Energy Model is commonly considered through the introduction of the energy efficiency factor which can be assigned either separately for both charging, η^{ch}, and discharging, η^{dis}, operations [86] or as a round-trip energy efficiency for the whole cycle [18, 87]. The generic Power-Energy

Model assumes fixed energy efficiencies and constant rated charging/discharging power that do not depend on SoE_t or the rate of charging/discharging current. The evolution of state-of-energy is a core of the Power-Energy Model and the relationship between two consecutive observations of SoE_t with a time step τ between them is expressed as:

$$SoE_t = SoE_{t-1} + \tau(\eta^{ch} ch_t - \frac{dis_t}{\eta^{dis}}). \tag{2.1}$$

The technical aspects of LIBESS are considered by enforcing limits on the charging and discharging maximum power and allowing only to store energy until the rated energy capacity is reached. Expression for state-of-energy (2.1) allows the schedule with simultaneous charging and discharging (e.g., that may be realized for electricity market cases with negative nodal energy prices or for ideal batteries with efficiencies equal to unity [88]). In this case, to avoid simultaneous charging and discharging, binary variables are introduced [89]. However, when the cost of LIBESS operation is included in the objective, energy efficiencies are less than unity, and a mixed-integer programming framework is not implemented, simultaneous charging and discharging is suboptimal and should not appear in the optimal solution [41, 87, 90]. The self-discharging rate coefficient is not added to equation (2.1) since this parameter is negligible and equal to 3-5% per month for the lithium-ion battery [91] and a battery is expected to have one full cycle per day. The Power-Energy Model can be updated by adding some features of the lithium-ion cell operation through the functional dependencies of maximum permissible charging/discharging power on state-of-energy as in [32, 35], or energy efficiency on state-of-energy and charging/discharging power as in [31, 37], or both dependencies as in [31, 33, 71]. A simple Power-Energy Model can also be coupled with degradation description of the battery as result of cycling or calendar ageing. In power system economics studies, degradation is mostly modelled either enforcing operational limits [44, 45], or using the energy throughput model [17], or employing the cycle-counting model [70]. The last two approaches can be included in the optimization framework by assigning the cost of degradation in the cost function or by limiting degradation through the introduction of additional constraints to a Power-Energy Model.

In the energy throughput or power-based method, there is a linear dependence between the energy capacity fade and the energy throughput [17, 45, 92, 93]. It is assumed that the amount of energy that can be stored and delivered by LIBESS throughout its lifespan is fixed. A battery is often defined as healthy until it reaches the End-of-life (EoL) state that occurs when the battery has lost 20% of the original capacity. The framework can be built by incorporating degradation cost in the objective [17] or by limiting the number of full charging/discharging cycles per day [44] or per year [45]. The energy throughput technique for ageing assessment works properly for one charging/discharging cycle per day [73]. The cycle-counting degradation model relies on the nonlinear ageing occurred from cycling: cycles with smaller depth-of-discharge (DoD) contribute less into the degradation of the battery [70]. The cycles are extracted from a state-of-energy profile using the rainflow cycle-counting algorithm [94]. Each cycle with a certain DoD is assigned with a fixed amount of degradation to the energy capacity according to the cycle depth ageing stress function that can be obtained from the experimental data. The cycle-counting method is incorporated into the optimization framework by including the cost of degradation into the objective function. This cost is calculated by benchmarking the amount of degradation with the battery replacement cost [42]. Although the cycle-based degradation model is more advanced than the energy throughput method, both techniques do not consider the effect of the average state-of-energy around which the charging/discharging cycle occurs [48]. Another limitation of the cycle-counting degradation model with rainflow algorithm is that it only has a recursive form. Several approximations suitable for the optimization environment were suggested [42, 95, 96]. Some authors also employed empirical nonlinear degradation models [48, 49] where the cumulative degradation cost function was constructed for different state-of-energy and the current rates for charge/discharge.

The energy efficiency and maximum power capacity of the LIBESS also degrades with cycling or when the battery ages over time [97]. The effect of ageing on the energy efficiency and maximum charging/discharging power was explored in [98] and [71]. A linear relationship between the fading capacity and maximum charging/discharging power was assumed in [71] and the growth of the cell internal resistance was explored in [98].

The incorporation of a generic Power-Energy Model within power system optimization frameworks usually leads to a linear programming problem [45] or a linear mixed integer programming problem [31] that can be easily solved with standard commercial solvers.

2.2.2 Voltage-Current Model

The charging/discharging schedule calculated using a Power-Energy Model may lead to the operation of the battery out of permissible range for current and voltage [32]. If this occurs, the "optimized" operation will be corrected by BMS [27]. This will lead to a deviation from estimated financial benefits and grid service commitment in power systems studies. The formulation of the battery model can be improved if some details of the battery operation are incorporated. A phenomenological model, such as the equivalent-circuit model, is designed to replicate the battery's charging/discharging performance and is usually used in BMS [99]. The description of LIBESS operation based on the electric circuit presents an attractive option to model the cell using the Kirchhoff equations.

The equivalent-circuit model by its nature does not model the dynamics of the internal processes inside the cell but characterizes the measurable response of the cell to the external influence. The charging/discharging performance curves show how the voltage, which is the state variable, across the cell changes with the current, which is the control variable, flowing through the cell while charging/discharging. With regard to the decision variables when an equivalent-circuit model is employed for the optimal control in the power system, the model can be referred to as a Voltage-Current Model. The impedance parameters of the Voltage-Current Model are obtained from fitting an experimental data or the manufacturer's specification to the governing equation of the suggested circuit model.

There are various configurations of an electric circuit for a Voltage-Current Model [100]; the choice depends on the accuracy requirement, the level of tolerance to the computational complexity, and the cell chemistry. The first-order approximation consists of two elements: voltage source and resistance [79]. A more advanced Voltage-Current Model usually consists of a set of resistors and capacitors in series or parallel, current sources, and special nonlinear elements. The simple electric circuit that captures the main processes in the cell is shown in Fig. 2.1b. This model was derived using [79] and is based on empirical observations. The variable voltage source changes its output as a function of state-of-charge. This voltage is sometimes referred to as an open-circuit voltage OCV_t [79] and is supplied by the electrode chemistry. The nonideality of the cell is modelled through resistor R_0. This resistor also ensures that the output voltage drops relatively to the open-circuit voltage when the load is connected, and increases above the open-circuit voltage during charging operation. The lithium ions do not immediately stop flowing when the charging/discharging is interrupted. To model this diffusion process, a resistor, R_d, and capacitor, C_d, in parallel are employed. The nonlinear elements are used to simulate the so-called hysteresis effect when an open-circuit voltage reaches different values for the same state-of-charge as a consequence of thermodynamic hysteresis or mechanical hysteresis [101]. The latter is a consequence of mechanical stress on electrodes from lithiation and delithiation and the former originates from the variation of the lithium intercalation rates between particles of active electrode material.

The control variable for the Voltage-Current Model is the current through the cell I_t. It is chosen to be positive during the discharge for consistency of the description. The state variables, in this model, are the state-of-charge SoC_t measured in Ah, the operating voltage V_t, and the diffusion voltage V_t^d, i.e., the voltage across a capacitor C_d. The evolution of the state-of-charge is given as:

$$SoC_t = SoC_{t-1} - \eta_c I_t \tau_{VCM} \tag{2.2}$$

where, τ_{VCM} corresponds to the time step between two estimates of SoC_t; and η_c stands for the coulombic efficiency that reflects how much charge is lost during the charging/discharging cycle.

Using Kirchhoff's Law for voltage, the following expression can be derived to relate voltages in the circuit [79]:

$$OCV_t(SoC_t) = I_t R_0 + V_t^d + V_t. \tag{2.3}$$

Using Kirchhoff's Law for current, the relationship for currents in a parallel RC branch is given as [79]:

$$I_t = \frac{V_t^d}{R_d} + C_d \frac{dV_t^d}{dt}. \tag{2.4}$$

If the derivative $\frac{dV_t^d}{dt}$ is approximated using finite differences, the diffusion voltage V_t^d can be calculated as:

$$V_t^d = \frac{R_d C_d}{\tau_{VCM} + R_d C_d} V_{t-1}^d + \frac{\tau_{VCM} R_d}{\tau_{VCM} + R_d C_d} I_t. \tag{2.5}$$

The Voltage-Current Model is formulated using the single cell perspective which assumes that all cells within the battery show the same performance [102]. Although the battery balancing scheme provided by BMS is intended to maintain variation between the cells of the battery pack at minimum [103], in general, this statement requires additional investigation [24, 104]. DC Voltage and current are not typical variables in power system economic studies, but both of these can be employed naturally to find the power P_t supplied or consumed by a LIBESS that consists of N lithium-ion cells in series and in parallel, as follows:

$$P_t = N I_t V_t. \tag{2.6}$$

The Voltage-Current Model allows for the restrictions specified by the producer of the lithium-ion cell in the box constraint on current and voltage, as follows:

$$V^{Min} \leq V_t \leq V^{Max} \tag{2.7}$$

$$-I^{MaxCh} \leq I_t \leq I^{MaxDis} \tag{2.8}$$

where, V^{Min} and V^{Max} identify operational limits for voltage; and I^{MaxCh} and I^{MaxDis} are maximum absolute values of continuous charging and discharging currents. The range of SoC_t is limited from one side by nominal capacity Q^{Max} in Ah, as follows:

$$0 \leq SoC_t \leq Q^{Max} \tag{2.9}$$

The model presented above is discussed in more detail in [79] and was used in the optimization framework by [102]. In contrast, Taylor *et al.* [36] used a simpler electric circuit composed of the voltage source and a resistor in their work to derive a strategic operation of LIBESS. Other electric circuits that can be used in optimization frameworks can be taken from [100]. The examples of the other equivalent-circuit models derived from the physics-based models can be found in [34, 105, 106]. The degradation can be included in the Voltage-Current Model using the energy throughput as in [102] or modelling the side reactions by means of additional elements in the equivalent circuit as in [106]. The Voltage-Current model can also be built without a reference to the underlying electric circuit and operates using empirical relationships. For instance in [19], the voltage of the lithium-ion cell, as a function of charging/discharging current and state-of-charge, was constructed using bi-variate cubic splines.

The incorporation of a Voltage-Current Model, which is governed by equations (2.2),(2.3),(2.5)-(2.8), into the optimization framework leads to a nonlinear programming problem because of a nonlinear relationship between open-circuit voltage and state-of-charge. The final problem can be solved with various off-the-shelf nonlinear solvers such as IPOPT [107] or using linearization techniques combined with the commercial linear solvers.

2.2.3 Concentration-Current Model

Despite having a number of advantages over the Power-Energy Model, the Voltage-Current Model does not provide information about the physical process inside the battery and can produce errors if it is used outside of the operating conditions for which it was empirically built [79]. In contrast, the physics-based electrochemical model of a lithium-ion cell can achieve better accuracy [102]. The enhanced model of a lithium-ion cell is able to characterize the transport of charge carriers, interfacial reactions, thermal effects, and their mutual effects on each other [79]. The most rigorous model is too complex for the optimization framework because the model contains coupled partial differential equations and nonlinear algebraic expressions [32].

The trade-off between accuracy and possibility to implement a more advanced model in the optimization framework can be found in the single particle model of the lithium-ion cell (Fig. 2.1c). The single particle model limits its consideration to the physical principles such as the transport of lithium in the active material of electrodes and the kinetics of the lithium intercalation/deintercalation reactions [108]. The model originates from the porous electrode theory [109], which is used to quantify electrode processes within the porous electrodes. The single particle model is built on several assumptions [110]. First, the active material of both electrodes is composed of uniform spherical electrode particles, which all have an equal radius R^i (the superscript i is replaced by p for positive electrode and it is changed to n for negative electrode). A single electrode particle is employed to simulate the transport of lithium in the active material of the electrode. Second, the concentration of the lithium ions in the electrolyte is assumed to be uniform and constant. Finally, the rate of electrode reaction at the electrode/electrolyte interface does not change from one electrode particle to another. The second and third assumptions are valid in cases of low to medium current through the cell [108] when the impact of the electrolyte potential is negligible [111].

The movement of lithium under the concentration gradient in the electrode particle with radius R^i is described by a one-dimensional parabolic partial differential equation in spherical coordinates, as follows [110]:

$$\frac{\partial c^i}{\partial t} = \frac{D^i}{r^{i2}} \frac{\partial}{\partial r^i}(r^{i2} \frac{\partial c^i}{\partial r^i}) \tag{2.10}$$

where, c^i stands for the concentration of lithium atoms in the electrode particle; r^i is a radial coordinate; and D^i is the diffusion coefficient of lithium in the electrode active material. The homogeneous Neumann boundary condition is applied at the center of the electrode particle to conserve symmetry, as follows [108]:

$$(D^i \frac{\partial c^i}{\partial r^i})_{r^i=0} = 0 \tag{2.11}$$

The molar flux of lithium ions, i.e., the reaction rate of the deintercalation/intercalation process, J^i on the surface of the electrode sets the Neumann boundary condition for the diffusion equation, as follows [112]:

$$(D^i \frac{\partial c^i}{\partial r^i})_{r^i=R^i} = -J^i. \tag{2.12}$$

The initial condition is defined as [110]:

$$(c^i(r^i, t))_{t=0} = c_0^i(r^i) \tag{2.13}$$

where, $c_0^i(r^i)$ stands for the initial concentration of lithium in the electrode. This concentration depends on the initial state-of-charge of the lithium-ion cell. The diffusion equation with the boundary conditions presents a challenge for incorporating it as a constraint in the optimization framework. The "optimization-wise" formulation can be derived through the finite differences of the original partial differential equations [79] or their approximations based on the ordinary differential equations [113, 114], or using the Chebyshev collocation method [108].

The electrode reaction is characterized by the Butler-Volmer kinetics equation [112]. This expression describes the rate of the electrode reaction, i.e., the molar flux of lithium ions, at which lithium ion consumes electron and converts to neutral atom inside the electrode or vice versa and is expressed as:

$$J^i = \frac{2j_0^i}{F}\sinh(\frac{F\eta^i}{2RT}) \tag{2.14}$$

where, F is the Faraday constant, R is the gas constant, and T is temperature. The activation overpotential η^i is responsible for driving the current that was generated at the electrode during the lithium intercalation/deintercalation process. The exchange current density j_0^i represents the oxidation and reduction currents without external impact and is given as:

$$j_0^i = k^i\sqrt{(c^{Max,i} - c^{\text{surf},i})c^{\text{surf},i}c^{\text{el}}} \tag{2.15}$$

where, k^i denotes the reaction rate constant; $c^{\text{surf},i}$ stands for the lithium concentration at the surface of the electrode particle; $c^{Max,i}$ is the maximum concentration of lithium atoms in the electrode particle; and c^{el} is the electrolyte concentration (constant for single particle model).

Another parameter to characterize the lithium-ion cell is the so-called equilibrium potential or the open-circuit potential of the electrode that shows how the Gibbs free energy changes when lithium ions enter/leave the electrode [115]. The functional dependence between the concentration of lithium on the surface of the electrode, $c^{\text{surf},i}$, and open-circuit potential, OCP^i, is determined experimentally for each type of electrode chemistry when there is no current flowing through the cell (equilibrium state). When the cell is charging or discharging, the potential of the electrode deviates from the open-circuit potential, and is known as the solid-phase potential, ϕ^i, and is expressed as:

$$\phi^i = \eta^i + OCP^i(c^{\text{surf},i}) \tag{2.16}$$

Finally, the single particle model relates the applied charging/discharging current with the rate of the electrode reaction through equation (2.17) for the positive electrode and equation

(2.18) for the negative electrode respectively, as follows:

$$J^p = -\frac{I_t R^p}{3\nu^p \varepsilon^p F} \tag{2.17}$$

$$J^n = \frac{I_t R^n}{3\nu^n \varepsilon^n F} \tag{2.18}$$

where, ε^p and ε^n denote the volume fraction of active material in the corresponding electrode; ν^p and ν^n are the volumes of each electrode; and I_t is the current through the lithium-ion cell.

Finally, the voltage of the lithium-ion cell is given as:

$$V_t = \phi^p - \phi^n. \tag{2.19}$$

From an optimization perspective, the single particle model [39, 102] introduces current and concentration as decision variables, thus it will be referred to in this work as the Concentration-Current Model. Similar to a Voltage-Current Model, the Concentration-Current Model represents only one lithium-ion cell and the projection of this model on the whole battery requires an assumption that all cells behave identically. The supplied and consumed power P_t by a battery composed of N lithium-ion cells is derived through applied current and the voltage across the cell:

$$P_t = N I_t V_t \tag{2.20}$$

The Concentration-Current Model allows introducing specifications of the cell in the box constraint form, as follows:

$$V^{Min} \leq V_t \leq V^{Max} \tag{2.21}$$

$$-I^{MaxCh} \leq I_t \leq I^{MaxDis} \tag{2.22}$$

where, V^{min} and V^{max} identify operational limits for voltage; and I^{MaxCh} and I^{MaxDis} are maximum continuous charging and discharging currents.

The capacity of the cell is constrained in the Concentration-Current Model through the lithium concentration in both electrodes:

$$c^{i,Min} \leq c_t^i \leq c^{i,Max} \tag{2.23}$$

where $c^{Min,i}$ and $c^{Max,i}$ are limits for lithium concentration in an electrode.

The state-of-charge is not employed in the Concentration-Current Model as a state variable, but it can be used for comparison with other battery models. It can be derived from the instantaneous lithium concentration in one of the electrodes, for example in the negative electrode [79], it is given as:

$$SoC_t = \frac{c_t^{\mathrm{surf},n} - c^{Min,n}}{c^{Max,n} - c^{Min,n}} Q^{Max} \tag{2.24}$$

where, Q^{Max} is the rated capacity of the lithium-ion cell.

When the Concentration-Current Model (2.10)-(2.23) is a part of the optimization framework, the whole decision-making problem is a nonlinear programming problem. This problem can be solved using a nonlinear commercial solver such as IPOPT [107].

The Concentration-Current Model can be naturally updated to include the physical description of the degradation [79]. The growth of SEI is selected as a principal contributor to the degradation process [116]. The SEI mathematical model employed here was taken from [110, 117]. The rate of the side reaction responsible for the formation of SEI is governed by the Tafel equation, as follows:

$$J^{\mathrm{sei}} = \frac{j_0^{\mathrm{sei}}}{F} \exp\left(\frac{F}{2RT} \eta^{\mathrm{sei}}\right) \tag{2.25}$$

where, η^{sei} is the overpotential of the side reaction; and j_0^{sei} stands for the exchange current for the side reaction. The overpotential η^{sei} is expressed as:

$$\eta^{\text{sei}} = \phi^n - OCP^{\text{sei}} - FJ^n Z^n \tag{2.26}$$

where, OCP^{sei} is the open-circuit potential of the side reaction; and Z^n is the resistance of the film on the surface of electrode. The total current through the negative electrode is composed of the intercalation/deintercalation current $J^{\text{Li},n}$ (J^n is replaced by this variable in equation (2.12)) and the side reaction current density J^{sei} and is given as:

$$J^{\text{sei}} + J^{\text{Li},n} = J^n \tag{2.27}$$

The resistance of the SEI film on the surface of the negative electrode Z^n increases as SEI forms [110] and is expressed as:

$$Z^n = Z^{0,n} + \frac{\delta^{\text{sei}}(t)}{\kappa} \tag{2.28}$$

where, $Z^{0,n}$ is the initial resistance of the layer on the surface of the negative electrode; δ^{sei} refers to the thickness of SEI film and κ is the ionic conductivity of SEI. It can be reasonably assumed that the rate of SEI growth is proportional to the rate of the side reaction [117] and is given as:

$$\frac{d\delta^{\text{sei}}(t)}{dt} = -\frac{J^{\text{sei}} M}{\rho} \tag{2.29}$$

where, M denotes the molar mass of SEI, ρ is the density of SEI. Equation (2.29) can be converted to the discretized version when including in the optimization framework. The increase in Z^n will lead to the decline in charging/discharging power. Finally, the loss in the lithium inventory due to the SEI formation during charging can be estimated as:

$$C_{loss} = -\int_{t_1}^{t_2} \frac{3\varepsilon^p \nu^n J^{\text{sei}}}{R^n} dt \tag{2.30}$$

where, $[t_1, t_2]$ is the time interval during which the cell was charging. Equations (2.25)-(2.30) can be included into nonlinear optimization frameworks. The Concentration-Current Model can be improved by adding description of the lithium-ion transport in electrolyte as in [118] to derive the optimal charging protocol or as in [119] for assessing revenue in the capacity market under given operation schedule.

2.2.4 Summary of the three reviewed lithium-ion battery models

The reviewed battery models are found to be employed in the decision-making problems that include stationary lithium-ion battery storage for power system level applications; those applications are discussed in the next section. These three models can be converted to one another: the Power-Energy Model can be seen as the Voltage-Current Model with constant voltage that is equal to the nominal voltage of the cell [19]; the Voltage-Current Model can be obtained from the Concentration-Current Model by matching the physical process inside the cell with the corresponding circuit component [34].

A simple Power-Energy Model is a system-level model of LIBESS and it can be used to describe any energy storage technology. This model relies on the system-level variables/parameters such as charging/discharging power, energy efficiency, and energy capacity. The emphasis on lithium-ion technology is performed by integrating the interdependence between variables/parameters of this model. The Voltage-Current Model and the Concentration-Current Model are built from the cell-level perspective. The Voltage-Current model is a phenomenological model and this modelling approach can be used for other battery technologies. The Concentration-Current Model is specially tailored for the lithium-ion batteries or for the batteries with similar concept of operation.

The main properties of each model from the system and optimization perspectives are classified in Table 2.1. Here, the term *dependence* has been applied to highlight the interdependence between system-level variables/parameters whereas the term *degrades* means that additional constraints can be added to characterize an ageing effect. The computational complexity increases from the Power-Energy Model to the Concentration-Current Model as

Table 2.1: System level characteristics of reviewed lithium-ion battery models and types of the corresponding optimization frameworks.

Battery model	**Energy efficiency**	**Charging Charging**	**Energy capacity**	**Degradation**	**Optimization technique**
Power-Energy Model	constant	constant	constant, degrades	Energy throughput, operational limits, cycle-counting	LP[1]
Voltage-Current Model	dependence	dependence	constant, degrades	Energy throughput, SEI	MILP[2], NLP[3]
Concentration-Current Model	dependence	dependence	constant, degrades	SEI	NLP

[1] Linear programming
[2] Mixed integer linear programming
[3] Nonlinear programming

a linear formulation transforms to nonlinear with a greater number of constraints [24]. The optimality in case of using the Voltage-Current Model and the Concentration-Current Model is not guaranteed. The linearization of these models can be done using a large set of binary decision variables. This is suitable for shorter optimization horizons [36] as the tractability may become an issue. Both Voltage-Current Model and Concentration-Current Model use either partial or ordinary differential equations in their formulations. In this case, more time steps within the intra-hour interval, which means more decision variables, are needed to improve the stability of the numerical solution. Moreover, the Power-Energy Model requires fewer parameters that can be easily taken from technical specifications provided by manufacturer [31]. Nonetheless, the Voltage-Current Model and the Concentration-Current Model provide the description of the processes inside the lithium-ion cell and, thus, more accurately describe LIBESS operation.

2.3 Alternative battery models in power systems studies

In this section, the publications in which optimal charging/discharging schedules were identified for different LIBESS applications are reviewed with the scope to define how LIBESS was modelled. The objectives of both system operators and independent storage owners are examined. The list of LIBESS applications is limited to system-level grid applications of LIBESS [16, 26], namely: economic energy arbitrage, frequency regulation, operating reserve, peak shaving, renewable integration assistance, and transmission upgrade deferral. Papers that are used in this section are classified by the models and the description of degradation in Table 2.2 and Table 2.3 respectively.

The database of studies was created based on the criteria for search that are given in Table 2.4. The search was done through the Scopus system using various combinations of terms from the first row of Table 2.4. We started by including all indexed journals and conferences but at the end, and after narrowing down the search, it was clear that the majority of relevant papers were published in the titles listed in the second row of Table 2.4. We also considered relevant references cited by the selected papers. The Power-Energy Model is the most widely used model; in our review, only a selected set of papers using this model are included and some papers that utilized this model without additional new discussion points were not included in the current review.

Current objective of various independent system operators is solely limited to develop a market model for the battery storage participation. The technical requirements are limited to the parameters of a simple power-energy model as the resource is usually a part for large-scale optimization for the day-ahead market, the real-time market, and the market for the ancillary services. For example, in California an optional end-of-hour state-of-charge bid parameter is introduced to their optimization framework to effectively operate the storage in the real-time market and to honour the commitment of the day-ahead and ancillary services schedule [120]. The constraints and contributions to the objective function are also highlighted for each LIBESS application that was considered.

This chapter gives a brief overview of selected papers and their case study. In the following section cross-evaluations and observations are presented and discussed.

Table 2.2: Literature survey on the battery grid applications with respect to the approaches for the battery modelling.

Application	Power-Energy Model	Voltage-Current Model	Concentration-Current Model
Energy arbitrage only	[17, 31–33, 38, 44, 45, 48, 50, 69, 92, 93, 98, 102, 121–125]	[102]	[38, 102]
Frequency regulation only	[70, 95, 125]		[39]
Energy arbitrage and frequency regulation	[35, 37, 46, 73, 126, 127]		
Energy arbitrage and operating reserve	[42, 49]		
Energy arbitrage, frequency regulation, and operating reserve	[18, 41, 96, 125, 128]		
Peak shaving	[24, 47, 129]	[24, 36]	[24]
Renewable integration assistance	[71, 130–132]	[19, 133]	
Transmission upgrade deferral	[20, 134–136]		

Table 2.3: Literature survey on the battery grid applications with respect to the degradation description.

Application	Without degradation	Empirical description	Physics-based formulation
Energy arbitrage only	[31–33, 69, 121–125]	[17, 44, 45, 48, 50, 92, 93, 98, 102]	[38, 102]
Frequency regulation only	[125]	[50, 70, 95]	[39]
Energy arbitrage and frequency regulation	[35, 126, 127]	[46, 73]	
Energy arbitrage and operating reserve		[42, 49]	
Energy arbitrage, frequency regulation, and operating reserve	[18, 41, 96, 128]	[41, 96]	
Peak shaving	[24, 36, 129]	[47, 129]	
Renewable integration assistance	[19, 130, 131]	[71, 132]	[133]
Transmission upgrade deferral	[20, 134–136]		

2.3.1 Economic energy arbitrage

Economic energy arbitrage is exploited by an independent LIBESS operator to generate revenue by charging the battery under the low-price conditions and by discharging back to the electric grid when prices are higher. The economic analysis of the energy arbitrage application of LIBESS was accelerated by the restructuring and deregulation in the electric

Table 2.4: Search criteria for the selection of manuscripts for review.

Search terms	Battery model
	Degradation
	Energy arbitrage
	Frequency regulation
	Operating reserve
	Peak shaving
	Renewable generation
	Transmission deferral
Source titles	Applied Energy
	Journal Of Energy Storage
	Journal Of Power Sources
	Energies
	IEEE Transactions On Smart Grid
	IEEE Transactions On Sustainable Energy
	IEEE Transactions On Power Systems
	IEEE Access
	IEEE Power And Energy Society General Meeting
	International Journal of Electrical Power and Energy Systems

utility industry, and one of the first works on this topic was done by Graves *et al.* [121]. The energy arbitrage problem is formulated as an optimization problem to maximize profit of the independent storage owner, or to minimize the cost of running the system from the perspective of the independent system operator. The contribution from LIBESS from taking advantage of the electricity price volatility to the objective cost function is expressed as follows [17]:

$$C_{EA} = \sum_{t=1}^{T_{EA}} \lambda_t^E \Delta\tau^{EA} (P_{dis,t}^{EA} - P_{ch,t}^{EA}) \tag{2.31}$$

where, $P_{dis,t}^{EA}$ and $P_{ch,t}^{EA}$ denote power discharged and charged respectively in the energy market; $\Delta\tau^{EA}$ is duration of time interval t and it is usually assumed to be equal one hour in reviewed power systems techno-economic studies; T_{EA} is a set of time intervals within the decision-making horizon; and, λ_t^E is an hourly electricity price.

Most works that estimate economic benefits of the energy arbitrage by LIBESS employ a simple Power-Energy Model. In [69], perfect information about price and demand and a price-taker model were used to assess the economic benefits of incorporating energy storage into the New York electricity market. The effect of large-scale energy storage on electricity price formation was examined in [122]. The strategic behavior of a LIBESS operator under price uncertainty in day-ahead and real-time electricity markets was addressed in [123]. Several studies [17, 45, 48, 92, 93] combined a Power-Energy Model with an empirical degradation model to estimate LIBESS profitability for energy arbitrage. The empirical based degradation formulation for the energy capacity with the assumption of linear dependence between energy throughput and extent of capacity fading significantly changed the cost-effectiveness of LIBESS investment [17]. In their LIBESS model, authors also incorporated the contribution to energy losses from the conversion and thermal systems through the constant efficiency factor. However, no conclusions regarding this improvement were reported in their case study. In [45], the analysis of energy arbitrage is performed with so-called equivalent full cycles. In their market settings, they demonstrated that an extended calendar life is more profitable than an extended cycle life. The LIBESS operator would choose charging/discharging cycles with greater arbitrage trading profit if a longer calendar life is possible. Maheshwari and co-workers [48] applied their own experimental data with lithium-ion cells to derive their nonlinear degradation model. They claimed that DoD combined with cycle life and energy throughput quantification techniques for degradation fails to acknowledge the impact of state-of-energy and applied current, which were employed in their work through linear interpolation of their experimental data. In [92], the optimal value of maximum charging/discharging power was selected for the fixed capacity considering its degradation over the battery lifespan. Mohsenian-Rad [44] introduced charging and discharging bidding strategies in a stochastic framework for self-schedule and economic bids. Using short-term marginal cost per unit of degradation, which was derived from energy throughput and capital cost of the battery, He *et al.* [93] obtained a more accurate estimate of the energy arbitrage business case for the California day-ahead electricity market. Overall, the energy arbitrage operation considering ageing of the battery gives a better estimate in the cost/benefit analysis, but methods to characterize ageing are completely empirical and the results were not validated with real experience.

Some attempts have been made in order to improve the accuracy of the Power-Energy Model description for LIBESS representation used in energy arbitrage. It included the functional dependence between energy efficiency, state-of-energy, and maximum charging/discharging power. Sakti *et al.* [31] updated a Power-Energy Model by considering the nonlinear dependence of the maximum charging/discharging power limits and energy efficiency on state-of-energy. Although the model was empirical by the formulation, authors affirmed that a simple Power-Energy Model of LIBESS may overestimate the earnings from energy arbitrage by 10% compared with their most sophisticated model for a more volatile price signal resolution over the 7-day decision horizon. The authors of [32] applied the results of their experimental findings to better define the limits of available charging power to reflect the constant-current/constant-voltage charging operation of the lithium-ion cell. The available charging power depends on the state-of-energy. If a generic Power-Energy Model is used for LIBESS characterization the optimal schedule in the energy arbitrage application may overestimate the profit by 300% compared with the actual output obtained from scaled laboratory LIBESS that executed an "optimal" schedule for their case study. Authors of [33] studied the optimal operation of LIBESS deployed in the IEEE-14 system to exploit arbitrage opportunities. Similar to [31], their LIBESS model was an upgrade of a simple Power-Energy Model where fixed parameters were replaced with state-of-energy dependent ones. The use of nonlinear dependence between energy efficiency, charging/discharging power limits and state-of-energy was justified by the Voltage-Current Model as suggested by [34]. Using empirical charging/discharging curves, authors concluded that for their case study a simplistic Power-Energy Model overestimated economic opportunities by 7% and resulted in the operation of the battery beyond the recommended operating range. He *et al.* [98] combined a simple Power-Energy Model and energy throughput method for degradation description to derive the economic EoL of LIBESS. The term economic EoL was used by He to refer to the stage of the LIBESS state-of-health where the profit opportunities are vanished. In his optimization protocol energy efficiency, power, and energy capacity declined over time and as a result of cycling. Hesse [50] demonstrated the impact of the battery ageing, power-dependent battery efficiency losses and power electronic efficiency losses on the strategic dispatch in the electricity markets. They modelled losses in the converter as a function of the alternating current supplied/consumed power by a battery using piecewise approximation. Depending on operating conditions, power electronics losses could constitute from 25% to 40% of the total operating costs.

The energy arbitrage application is also a favourable choice to verify the robustness of more detailed operation models of LIBESS. Reniers *et al.* [102] calculated economic benefits from energy arbitrage over one year of operation for three different battery models, i.e., a Power-Energy Model, a Voltage-Current Model and a Concentration-Current Model and three different degradation formulations. The authors compared these degradation descriptions with the experimental data and concluded that the concentration-current model was the most precise. They found that the energy arbitrage market participation strategy obtained for the Concentration-Current Model was considerably more profitable and with less degradation. In a more recent publication by the same authors [38] the optimal charging/discharging dispatch for energy arbitrage with Power-Energy Model and Concentration-Current Model were used to cycle lithium-ion cells in the laboratory conditions. The profit and the capacity loss were more accurately predicted by the Concentration-Current model. Moreover, physics-based approach for battery operation and ageing characterization reduced degradation by 30% and improved revenue by 20% compared with conventional Power-Energy Model with empirical degradation. It is worth noting that some papers do time shifting of energy but not necessarily for economic arbitrage. For example, energy storage may be used to store excess renewable energy and use it during future dry times [134]. Or, energy storage could be used for reliability reasons by storing energy during off-peak hours and release the energy during the peak hours to enhance system reliability [135]. Some of those applications are reviewed in later sections.

Table 2.5: Comparison of the literature on only economic energy arbitrage applications of LIBESS with respect to the battery modelling and optimization techniques.

Study	Battery model	Energy efficiency	Charging/ discharging power	Energy capacity	Degradation	Network	Optimization framework	Uncertainty	Optimization subhorizon in days
[121]	PEM[1]	constant	constant	constant	none	none	LP[4]	deterministic	24
[17]	PEM	constant	constant	degrades	Energy throughput	none	MILP[5]	deterministic	2
[122]	PEM	constant	constant	constant	none	none	MILP	deterministic	1
[123]	PEM	constant	constant	constant	none	none	MILP	stochastic	1
[45]	PEM	constant	constant	constant	none	none	LP	deterministic	365
[48]	PEM	constant	constant	constant	SoC and C-rate dependence	none	MILP	deterministic	0.5
[92]	PEM	constant	constant	degrades	Energy throughput	none	MILP	deterministic	365
[93]	PEM	constant	constant	degrades	Energy throughput	none	LP	deterministic	365
[44]	PEM	constant	constant	constant	Energy throughput	none	MILP	stochastic	1
[31]	PEM	dependence	dependence	constant	none	none	MILP	deterministic	7
[32]	PEM	constant	dependence	constant	none	none	LP	deterministic	1
[33, 124]	PEM	dependence	dependence	constant	none	yes	LP	deterministic	1
[98]	PEM	degrades	degrades	degrades	Energy throughput and cycle-counting	none	LP	deterministic	1
[38, 102]	CCM[2], VCM[3]	dependence	dependence	constant	SEI and Energy throughput	none	NLP[6]	deterministic	2
[50]	PEM	dependence	constant	degrades	Nonlinear energy throughput	none	MILP	deterministic	30

[1] Power-Energy Model
[2] Voltage-Current Model
[3] Concentration-Current Model
[4] Linear programming
[5] Mixed integer linear programming
[6] Nonlinear programming

The reviewed papers are summarized in Table 2.5 with respect to the battery modelling approaches discussed in Section 2.2 and characteristics of the optimization framework. Here, the optimization framework is classified by the network constraints, optimization formulations, presence of uncertainties, and the duration of the decision-making subhorizon. The latter has been applied to define the amount of time during which the individual optimization problem was solved. The same approach to classification of the reviewed papers will be employed in later tables.

2.3.2 Frequency regulation

Frequency regulation is one of the ancillary service products and it is needed to keep frequency within an acceptable range when there is a mismatch between supply and demand. The fast ramping capabilities of LIBESS make it a favourable choice for frequency regulation: for example, 75% of large-scale LIBESS power capacity in US is used for the balancing of momentary fluctuations in the system [137]. Depending on the structure of particular electricity markets, the frequency regulation products can be traded in the day-ahead or real-time markets [18]. If the independent system operator procures the frequency service product from the electricity market participants, it means that a market participant is required to increase (regulation up) or to decrease (regulation down) its power output to comply with the sold obligations. The frequency regulation service provider is compensated through a two-part structured payment as it was requested by recent regulations in the US [138] to fairly treat resources with fast ramping capability. The first part is paid for the provision of the capacity for frequency regulation and is referred to as capability payment whereas the second part is the performance payment. The market for the frequency regulation product can be single, i.e., the output can be changed in both directions(e.g., in Alberta [139]), or separate markets for regulation up service and regulation down service (e.g., in California [139]). The costs/revenues associated with procuring/providing is added to the objective function of the optimizer and is expressed as follows [18, 127]:

$$C_{FR} = \sum_{t=1}^{T_{FR}} [\lambda_t^{RU} P_t^{RU} + \lambda_t^{RD} P_t^{RD} + \rho_t (P_t^{RU} + P_t^{RD}) + \lambda_t^{E} \sum_{r=1}^{T_{FR,1h}} (P_{t,r}^{RUd} - P_{t,r}^{RDd}) \Delta\tau_{T_{FR,1h}}] \quad (2.32)$$

where, T_{FR} is a set of time intervals within the decision-making horizon; λ_t^{RU} and λ_t^{RD} are frequency regulation up and down market capability clearing prices; P_t^{RU} and P_t^{RD} stand for capacity committed to regulation up and down respectively; ρ_t is the performance price in regulation; λ_t^{E} is the real-time electricity price; $T_{FR,1h}$ is a set of time intervals within the intra-hour interval to perform frequency regulation; $\Delta\tau_{T_{FR,1h}}$ is duration of time interval r

and, $P_{t,r}^{RUd}$ and $P_{t,r}^{RDd}$ stand for the actual capacity provided for the regulation up and down within one hour.

The frequency regulation application of LIBESS in power system economics studies is often combined with other services. The energy arbitrage application (Table2.6) is a common pair for the frequency regulation application. The LIBESS is mostly modelled through a generic Power-Energy Model [126, 127] for charging/discharging performance whereas the degradation is characterized by means of an empirical relationship [46, 70, 73, 95, 96]. Byrne *et al.* [126, 127] explored profitability of energy storage in various energy and frequency regulation markets in America. Xu [70] found the optimal control policy for LIBESS deployed in their case study to boost profit from the performance-based frequency regulation market using a chance-constraint optimization. The author used the cycle counting algorithm to characterize the long-term performance. The optimal bidding strategy in the frequency regulation market for the electric vehicle aggregator with different participation scenarios was outlined in [35]. Their model was able to simulate the transition from constant current mode to constant voltage mode of charging operation. They highlighted that their representation of the lithium-ion battery resulted in a more accurate estimate of financial benefits: there was up to 20% difference compared with a generic Power-Energy Model associated with LIBESS. Shi and co-workers [95] coupled a Power-Energy Model with three different degradation models, namely, the fixed cost of degradation, the energy throughput method, and cycle-based model based on the rainflow algorithm, to explore the financial benefits of frequency regulation for the LIBESS owner in the their case study. It was shown that the rainflow cycle-based degradation model projects up to 27.6% growth in revenue, and thus a greater return on investment, and almost 85% increase in battery life expectancy. In [73], a Power-Energy Model coupled with the energy throughput ageing quantification technique was used to find the optimal energy capacity of LIBESS, which profits from energy arbitrage and frequency regulation with compensation for capacity and energy provided in the California day-ahead and real-time energy and ancillary services markets. Assuming a constant degradation rate, the loss of capacity was directly incorporated into the operation framework as a constraint. Reference [46] proposed a robust optimization framework to calculate strategic operation of LIBESS in joint frequency regulation and energy markets while considering ageing of the battery though the rainflow algorithm. Nguyen *et al.* [37] replaced the fixed energy efficiency of a generic Power-Energy Model with one that nonlinearly depends on the charging/discharging power and state-of-energy. The parameters for their empirical model were calculated from the charging/discharging curve provided by the cell manufacturer. The proposed nonlinear model estimated almost 17% less of the total revenue over one year compared with simple Power-Energy Model if it was installed in their market environment.

In [39], a Concentration-Current Model was employed to find the optimal schedule of LIBESS for the frequency regulation market. The strategy was compared with one obtained using a Power-Energy Model with degradation cost, which was proportional to capacity committed to frequency regulation, in the objective function and with one where degradation was calculated using the SEI method in postprocessing of the optimal schedule. The authors reported a 143% increase in lifetime and 35% growth in profit compared to a generic Power-Energy Model.

The reviewed papers are classified in Table 2.6 with respect to the battery modelling approaches discussed in Section 2.2 and characteristics of the optimization framework.

2.3.3 Operating reserve

The operating reserve services is intended for the grid frequency management if a significant unpredictable deviation to the supply/demand balance occurs in the system. Operating reserves are usually divided into spinning and non-spinning products. The spinning reserve is provided by resource, which is online and supplies power to the grid, and is capable to increase its output. The non-spinning reserve is procured from the units that are usually offline but can be brought online with a short notice. The minimum amount of the procured

Table 2.6: Comparison of the literature with the frequency regulation application of LIBESS with respect to the battery modelling and optimization techniques.

Study	Application	Battery model	Energy efficiency	Charging/ discharging power	Energy capacity	Degradation	Optimization framework	Uncertainty	Optimization subhorizon in days
[70]	FR[1]	PEM[3]	constant	constant	constant	Cycle-counting	LP[5]	chance-constrained	1
[125]	FR	PEM	constant	constant	constant	none	MILP[6]	robust	1
[95]	FR	PEM	constant	constant	constant	none	MILP	deterministic	0.083
[39]	FR	CCM[4]	depend.	depend.	degrades	SEI	NLP[7]	deterministic	0.083
[126], [127]	EA[2]+FR	PEM	constant	constant	constant	none	LP	deterministic	30
[35]	EA+FR	PEM	constant	depend.	constant	none	LP	stochastic	1
[73]	EA+FR	PEM	constant	constant	degrades	Energy throughput	LP	deterministic	1825
[46]	EA+FR	PEM	constant	constant	constant	Cycle-counting	LP	robust	1
[37]	EA+FR	PEM	depend.	constant	constant	none	heuristic	deterministic	1

[1] Frequency regulation
[2] Economic energy arbitrage
[3] Power-Energy Model
[4] Concentration-Current Model
[5] Linear programming
[6] Mixed integer linear programming
[7] Nonlinear programming

capacity for operating reserve is defined by power system reliability standards, and it is traded through the operating reserve market. The optimal schedules for LIBESS are determined through an optimization framework that minimize/maximize the costs/revenues associated with procuring/providing operating reserves from a merchant storage operator. A typical objective function for this service is given as follows [18]:

$$C_{OR} = \sum_{t=1}^{T_{OR}} [\lambda_t^S P_t^S + \lambda_t^{NS} P_t^{NS} + \lambda_t^E \Delta\tau_{OR}(P_t^{Sd} + P_t^{NSd})] \tag{2.33}$$

where, T_{OR} is a set of time intervals within the decision-making horizon, λ_t^S and λ_t^{NS} are spinning and non-spinning reserve clearing prices, P_t^S and P_t^{NS} stand for capacity committed to spinning and non-spinning reserves respectively,λ_t^E is the real-time electricity price, $\Delta\tau_{OR}$ is duration of time interval t, $T_{FR,1h}$ is a set of time intervals within the intra-hour interval to perform frequency regulation, and P_t^{Sd} and P_t^{NSd} stand for the actual capacity provided for the spinning and non-spinning reserve services within one hour.

The operating reserve revenue stream for the LIBESS owner is usually considered as an additional source of revenue and it is bundled with other LIBESS applications in power system economic analysis [18]. The strategic operation of LIBESS that provides operating reserve services is usually derived with a simple Power-Energy Model without description of degradation such as in [125, 128] or including ageing impact as in [18, 42, 49, 96]. In [128], it was shown that the strategic approach of an independent energy storage owner in the energy and ancillary services markets facilitates higher penetration of renewable generation. The robust optimization framework was employed to deal with uncertainty in market prices, deployment occurrence, and energy exchange for frequency regulation in [125]. In [18], fixing number of cycles per day to one, the authors analyzed strategic scheduling of LIBESS assuming that it is a price-taker in the energy market and a price-maker in the market for ancillary services. Xu *et al.* [42] proposed a dispatch strategy for LIBESS considering the cost of battery degradation that was formulated using the Rainflow cycle counting algorithm. In [49], the optimal strategy for LIBESS operator that submits the bids into both the energy and operating reserve market was derived by combining the impact of DoD and the discharge rate in the degradation cost function. Reference [96] modelled optimal market participation of LIBESS in three day-ahead markets: energy, frequency regulation and operating reserve markets. The profit of LIBESS was calculated on a daily basis and prorated by the number of the battery's daily equivalent 100%-DoD cycles. Perez *et al.* [41] examined the impact of applying practical box constraints on state-of-energy to limit degradation on the financial potential of LIBESS providing several services including the operating reserve. Although there was a drop in revenue from energy arbitrage, the net revenue has increased from operating reserve and frequency regulation contributions because of extended lifespan.

The reviewed papers are classified in Table 2.7 with respect to the battery modelling approaches discussed in Section 2.2 and characteristics of the optimization framework.

Table 2.7: Comparison of the literature with the operating reserve application of LIBESS with respect to the battery modelling and optimization techniques.

Study	**Application**	**Battery model**	**Energy efficiency**	**Charging/ discharging power**	**Energy capacity**	**Degradation**	**Optimization framework**	**Uncertainty**	**Optimization subhorizon in days**
[42]	EA[1]+OR[2]	PEM[4]	constant	constant	constant	Cycle-counting	MILP[5]	deterministic	1
[49]	EA+OR	PEM	constant	constant	constant	Cycle-counting and C-rate dependence	MILP	deterministic	1
[18]	EA+FR[3]+ OR	PEM	constant	constant	constant	none	MILP	stochastic, robust	1
[128]	EA+FR+ OR	PEM	constant	constant	constant	none	MIQCP[6]	deterministic	1
[125]	EA+FR+ OR	PEM	constant	constant	constant	none	MILP	robust	1
[96]	EA+FR+ OR	PEM	constant	constant	constant	Cycle-counting	NLP[7]	stochastic	1
[41]	EA+FR+ OR	PEM	constant	constant	degrades	Operational limits	MILP	deterministic	7

[1] Economic energy arbitrage
[2] Operating reserve
[3] Frequency regulation
[4] Power-Energy Model
[5] Mixed integer linear programming
[6] Mixed integer quadratically constrained program
[7] Nonlinear programming

2.3.4 Demand peak shaving

If a LIBESS is installed on the load side it could also work as a peak shaver to minimize the total electricity bill as a system operator can set a fixed price on the maximum power consumed over selected period in the form of demand charges. The strategic dispatch of LIBESS under these conditions is determined when the following term is added to the objective function [129]:

$$C_{PS} = \lambda_{Peak} P^{peak} \tag{2.34}$$

where, λ_{Peak} is the charge for the maximum power consumed and P^{peak} stands for the maximum power supplied by the electric grid.

There are several works where charging/discharging decisions were found for the peak shaving application. Braeuer [129] developed the optimization framework with a generic power-energy model to evaluate economic value of LIBESS when pairing with various industrial loads in Germany. Economic energy arbitrage, peak shaving, and primary control reserve are considered as revenue streams to decrease the overall cost for the load. Schneider *et al.* [47] investigated a strategic investment into LIBESS for a bundled peak shaving and energy arbitrage business model. Their optimization framework included Power-Energy Model, Rainflow cycle counting paradigm for battery degradation and it was solved heuristically through three stages: on the first stage, the daily scheduling maximizes energy arbitrage revenue corrected by a degradation penalty term, on the second stage the total monthly revenue from peak shaving and energy arbitrage is calculated, the third stage is used to define the optimal schedule over the year. Taylor [36] employed Voltage-Current Model formulation for LIBESS and compared it with Power-Energy Model. The parameters of the Voltage-Current Model were measured from their own lab experiments with lithium iron phosphate battery cells. First, the accuracy of the model was demonstrated by comparison with the experiment. Second, the optimal schedule of LIBESS based on the Voltage-Current Model formulation outperformed the results with Power-Energy Model when the optimal schedule of each model was processed by the battery hardware simulation tool. Although simulation was carried out at only two fixed levels of the current rate, it was clear that a generic Power-Energy Model model did not ensure reliable performance. In the review of battery models for the optimal control [24], the control strategy for LIBESS installed to reduce the total electricity bill over 24-hour decision horizon was obtained for three different battery models, namely a Power-Energy Model, the Voltage-Current Model and the Concentration-Current Model. The cost reduction in the bill was conducted using energy arbitrage and peak shaving applications of LIBESS. The degradation of the lithium-ion cell was not a part of the analysis. Although the net reduction in the electricity bill was almost the same for all models and stood at about 8%, the authors claimed that the control strategy for the Power-Energy Model was likely infeasible. The Voltage-Current Model and Concentration-Current Model gave similar results for the state variables such as voltage and current. The authors also used quadratic dependencies between direct current and alternating current powers supplied/provided by the

Table 2.8: Comparison of the literature with the peak shaving application of LIBESS with respect to the battery modelling and optimization techniques.

Study	Battery model	Energy efficiency	Charging/ discharging power	Energy capacity	Degradation	Optimization framework	Uncertainty	Optimization subhorizon in days
[129]	PEM[1]	constant	constant	constant	Energy throughput	LP [4]	deterministic	365
[47]	PEM	constant	degrades	degrades	Cycle-counting and Energy throughput	MILP[5], NLP[6]	deterministic	1
[36]	VCM[2]	depend.	depend.	constant	none	MILP	deterministic	1
[24]	CCM[3]	depend.	depend.	constant	none	NLP	deterministic	1

[1] Power-Energy model
[2] Voltage-Current Model
[3] Concentration-Current model
[4] Linear programming
[5] Mixed integer linear programming
[6] Nonlinear programming

battery to model the conversion efficiency. However, the impact of this improvement was not addressed. Additionally, the Voltage-Current Model was also combined with a temperature model to incorporate losses associated with heating ventilation and air conditioning systems for keeping the temperature within a defined temperature range. Such model increased the total electric bill by 0.11% compared with a baseline Concentration-Current Model.

The reviewed papers are classified in Table 2.8 with respect to the battery modelling approaches discussed in Section 2.2 and characteristics of the optimization framework.

2.3.5 Renewable integration assistance

LIBESS can also accelerate the integration of intermittent renewable capacity to the grid by mitigating its natural fluctuation and can increase the return on investment in a renewable generation project if it is combined with a LIBESS [137]. The objective of the optimization problems with this application can be either finding the optimal operation dispatch for the hybrid plant or the planning problem where the optimized LIBESS size is explored to maximize return on investment over the projected lifespan of a battery.

Similar to operation studies with other LIBESS applications, the renewable integration assistance application of LIBESS is mostly modelled with a simple Power-Energy Model [130, 131]. In [130] the size and optimal dispatch were determined for LIBESS paired with a wind farm. The solution enhanced the operational stability and economic feasibility of the wind power project. Bhattacharjee *et al.* [131] used a generic Power-Energy Model to optimally size energy storage and transmission interconnector, which were coupled with a wind power facility, for the strategic participation in the energy market. Recently more works [71,132] have been presented with LIBESS models that can ensure reliable performance and characterize capacity and power fading. Using a heuristic algorithm Shin [132] investigated the impact of LIBESS size on degradation while searching for the optimal LIBESS capacity supplementing photovoltaic generation for two scenarios of battery use: constant usable energy capacity and a fixed DoD. Jafari [71] studied the economic impact of pairing offshore wind farm with LIBESS. This model of LIBESS included varying energy efficiency and power limits. Calendar and cycling ageing of capacity were also incorporated in the model by a linear decline assumption for calendar ageing and combination of the energy throughput with the number of equivalent full cycles for cycling ageing respectively. The revenue from the optimal schedule with enhanced Power-Energy Model without degradation was 4% less than for the schedule obtained with a simplistic Power-Energy Model. When one of the degradation models was added to the optimization framework the estimated revenue decreased by 35%. The Voltage-Current model was employed in [19] to determine the optimal schedule of LIBESS over a 36-hour optimization horizon while minimizing the electricity bill of the user with on-site photovoltaic generation. Moreover, the converter losses were modelled as a function of alternating current power using a cubic spline approximation. The authors showed that this model avoids unsafe operation compared to the Power-Energy Model. Li [133] determined the ratings of LIBESS to improve dispatchability of the hybrid storage and wind farm plant employing the physics-based the Voltage-Current Model. The problem was solved using a developed particle swarm optimization algorithm.

The reviewed papers are classified in Table 2.9 with respect to the battery modelling

Table 2.9: Comparison of the literature with the renewable integration assistance application of LIBESS with respect to the battery modelling and optimization techniques.

Study	Battery model	Energy efficiency	Charging/ discharging power	Energy capacity	Degradation	Optimization framework	Uncertainty	Scope	Optimization subhorizon in days
[131]	PEM[1]	constant	constant	constant	none	MILP[3]	stochastic	planning	7
[132]	PEM	constant	constant	degrades	Cycle-counting and Energy throughput	heuristic	deterministic	planning	5475
[71]	PEM	depend.	depend.	degrades	Cycle-counting and operational limits	MILP	deterministic	operation	365
[19]	VCM[2]	depend.	depend.	constant	none	NLP[4]	deterministic	operation	1.5
[133]	VCM	depend.	depend.	degrades	SEI	heuristic	deterministic	planning	1

[1] Power-Energy model
[2] Voltage-Current Model
[3] Mixed integer linear programming
[4] Nonlinear programming

approaches discussed in Section 2.2 and characteristics of the optimization framework.

2.3.6 Transmission upgrade deferral

Another LIBESS application that brings significant changes to how the long-term planning of the power system is performed, is deferral or replacement of the traditional power system infrastructure – transmission lines. When LIBESS is installed downstream of a congested transmission corridor it can relieve congestion by discharging to meet the additional demand from the load. This is why, LIBESS is considered as a virtual transmission for the future grid. The strategic deployment of LIBESS can increase the asset utilization rate in the grid if it is planned correctly [140].

The class of planning problems from the system operator perspective, where the optimal size of LIBESS and its location in the grid are determined, is usually solved with the objective to minimize the sum of the capital cost of LIBESS and the operating costs of the system. A simple Power-Energy Model without degradation is usually incorporated into these optimization problems. For example, in [134], a static investment model was used to find siting and sizing decisions within the Western Electricity Coordinating Council inter-

Table 2.10: Comparison of the literature with the transmission upgrade deferral application of LIBESS with respect to the battery modelling and optimization techniques.

Study	Battery model	Energy efficiency	Charging/ discharging power	Energy capacity	Degradation	Optimization framework	Uncertainty	Scope	Optimization subhorizon in days
[134]	PEM[1]	constant	constant	constant	none	MILP[2]	stochastic	planning	1
[135]	PEM	constant	constant	constant	none	MILP	stochastic	planning	1
[136]	PEM	constant	constant	constant	none	MILP	deterministic	operation	1
[20]	PEM	constant	constant	constant	none	LP [3]	stochastic	planning	1

[1] Power-Energy model
[2] Mixed integer linear programming
[3] Linear programming

connection by means of the stochastic programming. Falugi and co-workers [135] studied the dynamic planning problem of the joint transmission and LIBESS deployment in the IEEE 118-bus system for the planning horizon of 16 years. The optimal decision plan was updated every four years.

The LIBESS that provides transmission services should be paid through the rate-based compensation. However, if LIBESS also provides other services to the grid it should be additionally compensated through the market. Such multiple service operation of LIBESS and corresponding compensation scheme currently face several regulatory barriers. The market model and corresponding policies for storage as a transmission asset are investigated by several utilities [141]. The operation strategy for energy storage that provided congestion relief service and also obtained revenue from energy arbitrage is examined in [136]. The optimal premium paid to the LIBESS owner as a rate-based compensation to relieve congestion is explored in [20]. Both papers utilized a generic Power-Energy Model without degradation.

The reviewed papers are classified in Table 2.10 with respect to the battery modelling approaches discussed in Section 2.2 and characteristics of the optimization framework.

2.4 Summary and concluding remarks

The previous sections have presented the current state of the lithium-ion battery modelling in power systems techno-economic studies and justified the need for additional investigation. First, three LIBESS models with different level of details that include both operational characteristics and degradation processes were reviewed. Their governing equations in appropriate format for the optimization framework were presented. The review of research papers where optimal operation and planning decisions were derived for the business cases with lithium-ion battery storage for various transmission system-level applications was performed. The classification of reviewed studies was carried out based on the LIBESS applications, battery models, and optimization techniques.

The system-level operational and planning studies predominantly employed generic Power-Energy Models to characterize the LIBESS charging/discharging performance and to quantify degradation as it can be seen from Tables 2.5-2.10. The reason for this is the simplicity and linearity of Power-Energy Models. However, starting in year 2018, models that describe the dynamics of the processes inside the lithium-ion battery by either the Voltage-Current Model or the Concentration-Current Model have started to appear in the power system studies literature in 2018 [102], in 2019 [24], and in 2020 [19, 36, 38, 39, 133].

Several authors [31–33, 35, 37] enhance a simplistic Power-Energy Model with the functional dependencies between energy efficiency, maximum charging/discharging power and state-of-energy to better model typical characteristics of the lithium-ion cell. The linear approximation was applied for all mentioned relationships to make them solvable for the optimization problems used in those studies. However, only in the case of [31] the final problem was a mix-integer linear problem whereas authors of [32, 33, 35] finished with a linear programming problem. The energy arbitrage application was used for the assessment of LIBESS models from [31–33] whereas the frequency regulation service revenue stream was assessed in [35]. The common drawback for these models is that they are phenomenological by their nature: limited experimental data were used to fit their mathematical models for selected operating conditions. Moreover, the degradation of LIBESS was not considered as only charging/discharging performance was an objective for the improvement.

An increasing number of studies for different LIBESS applications such as [48] for energy arbitrage, [47] for peak shaving, [70] for frequency regulation, and [49] for operating reserve showed that the economic viability of the project with LiBESS is not overestimated if the degradation models were used. However, various empirical degradation formulations, which are limited by their formulation, were used in the mentioned works.

The Voltage-Current Model was employed to assess energy arbitrage [102], peak shaving [36, 102], and renewable integration assistance [19, 133] applications only. Compared to the Power-Energy Model, this formulation ensure that the system-level variables and parameters such as energy efficiency, charging/discharging power are related.

Among three models to simulate the charging/discharging profile, the Concentration-Current Model can be seen as the most promising since it characterizes the dynamics of physical processes inside the cell and can be coupled with the physics-based degradation model such as SEI formation. The cost-benefit analysis of LIBESS with Concentration-Current Model was performed only for a discrete battery application such as energy arbitrage in [102], frequency regulation [39], and peak shaving [24]. The co-optimization of various LIBESS applications was not considered when this model is employed. This high-fidelity model was also not used for optimal sizing of LIBESS for the transmission services or renewable integration assistance.

There are several sources of concern for the application of the detailed lithium-ion battery models in power systems decision-making process. The first is that all studies with advanced battery models were run over the narrow optimization horizon of one to two days. This approach may over/underestimate the feasibility of the project. Secondly, the optimization frameworks with the Voltage-Current Model or the Concentration-Current Model require nonlinear optimization solvers or the heuristic strategy to tackle the problem. This does not guarantee a global solution and in general is computationally expensive to solve. An additional point regarding most of the reviewed studies with detailed models is a lack of network system constraints, perhaps to avoid computational complexity. The computational complexity of the detailed models also limits their use when sources of uncertainty exist.

Despite the differences in the reviewed papers, Table 2.11 and Table 2.12 is an effort to summarize the studied references that have provided some form of comparison when using different lithium-ion battery models. It can be concluded that advanced battery models can provide more accurate estimates for the economic potential of LIBESS, feasible charging/discharging schedule, and a more precise projection of the capacity and charging/discharging power fading.

The LIBESS, as well as other energy storage technologies applications by the corresponding duration of the provided service, are historically divided into the energy applications, where product is supplied for hours and minutes, and power applications, where time-scale of seconds and minutes is used [27]. The energy application encompasses economic energy arbitrage, operating reserve, renewable integration assistance, and transmission upgrade deferral whereas the examples of the power applications are frequency regulation and demand peak shaving. The impact of each service on the operation depends on the proposed optimization framework including the market model and the battery model and the corresponding parameters of the battery model and the case study. The study covering this topic is scarce and should be addressed in further investigations as only limited observations are reported in the literature. For example, Reniers [38] in his work with the energy arbitrage application revealed that higher state-of-energy are inherent to the optimal schedule with a simple Power-Energy Model compared to low levels of the Concentration-Current Model. Elliott *et al.* [142] experimentally proved that the rate of degradation for the energy arbitrage application is twice faster than for the frequency regulation service. Hesse [1] reported on the substantial difference in operation between frequency regulation and peak shaving services when they were compared based on the statistical distribution of values over the modelling interval for state-of-energy and charging/discharging power.

Based on these observations and considering data from Tables 2.5-2.10, several directions are suggested for future development:

- The impact of the detailed model of LIBESS without degradation on the profit-

Table 2.11: Classification of reviewed studies with respect to conclusion (Part 1).

Study	**Application**	**Battery model**	**Additional features**	**Validation**	**Reporting improvements**
[17]	Energy arbitrage	PEM[1]	degradation	comparison with a simple PEM	12–46% reduction in revenue
[48]	Energy arbitrage	PEM	degradation	comparison with Energy throughput method	44% error in degradation estimation
[93]	Energy arbitrage	PEM	degradation	comparison with a simple PEM	25% increase in revenue over lifespan
[31]	Energy arbitrage	PEM	interdependence	comparison with a simple PEM	10% reduction in revenue
[32]	Energy arbitrage	PEM	interdependence	comparison with an experiment	184% increase in revenue
[33]	Energy arbitrage	PEM	interdependence	comparison with a simple PEM	7% reduction in revenue
[102]	Energy arbitrage	CCM[2]	N/A	comparison with a simple PEM	175% increase in profit
[70]	Frequency regulation	PEM	degradation	comparison with a simple PEM	12-163% increase in profit over lifespan
[95]	Frequency regulation	PEM	degradation	comparison with Energy throughput	28% increase in profit over lifespan
[73]	Energy arbitrage and frequency regulation	PEM	degradation	comparison with Energy throughput	20% reduction in revenue
[39]	Frequency regulation	CCM	N/A	comparison with Energy throughput	38% increase in profit over lifespan
[96]	Energy arbitrage and frequency regulation and operating reserve	PEM	degradation	comparison with Energy throughput	29% increase in profit over lifespan
[49]	Energy arbitrage and operating reserve	PEM	degradation	comparison with a simple PEM	25% reduction in revenue
[49]	Energy arbitrage and frequency regulation and operating reserve	PEM	degradation	comparison with a simple PEM	44% increase in profit over lifespan
[50]	Energy arbitrage	PEM	degradation	comparison with a simple PEM	36% reduction in revenue
[36]	Peak shaving	VCM[3]	N/A	comparison with a simple PEM	The operation schedule is verified through experiment
[24]	Peak shaving	CCM	without SEI	comparison with a simple PEM	0.15% increase in profit

[1] Power-Energy model
[2] Concentration-Current model
[3] Voltage-Current Model

Table 2.12: Classification of reviewed studies with respect to conclusion (Part 2).

Study	Application	Battery model	Additional features	Validation	Reporting improvements
[71]	Renewable integration assistance	PEM	degradation and interdependence	comparison with a simple PEM	35% reduction in revenue
[37]	Energy arbitrage and frequency regulation	PEM	interdependence	comparison with a simple PEM	16% reduction in revenue
[38]	Energy arbitrage	CCM	N/A	comparison with a simple PEM	70% increase in profit over lifespan

[1] Power-Energy model
[2] Concentration-Current model
[3] Voltage-Current Model

maximizing operation of the energy storage for various grid applications was quantified by a few researchers. However, there is no consensus on how a more detailed model is crucial for short-term operation. For example, in [32], a simple Power-Energy Model overestimated the profit by 300%, 4% was demonstrated in [71], and no difference was stated by [38].

- An economic and technical feasibility study with either the Concentration-Current Model or the Voltage-Current Model was conducted for only one grid service. The analysis for the case of several stacked applications of LIBESS were not researched with these models before.

- Most of the grid-connected LIBESS at the transmission level in electrical power system studies is modelled through the cell-level and system-level perspectives. So improvements to the LIBESS model for operation and planning studies can be done through the inclusion of other components of LIBESS such as the energy conversion system, the battery management system, and the thermal management system.

- There is no discussion within the reviewed papers on which model type is best suited to evaluate the energy or power-related grid applications, as these must consider different technical and/or market requirements and protocols.

- The experimental data and field data of LIBESS in operation would be needed to benchmark the results of the optimal schedule obtained with more detailed models since currently only a few studies [32, 36, 38] verified their models with the experiment.

- The Concentration-Current Model has never been considered for planning studies as the system-level planning studies predominantly employed a generic Power-Energy model to characterize the LIBESS charging/discharging performance. As the lifespan of the lithium-ion cell component of a LIBESS is a quarter or half of traditional transmission and generation assets, the integration of LIBESS into the grid requires a multistage planning approach, where a replacement schedule is a part of the implementation plan and investment. The long-term multistage battery planning with replacement is completely out of consideration in the literature.

- The increased number of variables and constraints in the optimization framework brought by voltage-current and concentration-current models should be tackled with parallel computing as it was performed for a longer decision-making horizon with a Power-Energy Model considering degradation in [73].

- The stochastic formulation of the strategic operation of LIBESS is a computationally expensive problem by itself. The need in using a more detailed battery model for this optimization framework should be justified.

- A highly efficient, time-saving algorithm is needed for the nonlinear optimization problem of the planning and scheduling of the grid level applications if a sophisticated physics-based lithium-ion model, such as the Concentration-Current Model, is employed.

Chapter 3

Linearized Physics-Based Lithium-ion Battery Model for Power System Economic Studies[1]

3.1 Introduction

The majority of power system techno-economic decision-making studies utilize a simple power-energy model to simulate lithium-ion battery operation and various phenomenological descriptions for degradation [22, 30]. The rising number of simulation and experimental studies [32, 36, 102] indicates that a simple battery model can overestimate the economic potential of the project and result in charging/discharging profiles that violate the safe operating regime. The situation can be improved if a more detailed battery model is considered. This can be conducted either by adding details of the operational characteristics of LIBESS to the power-energy model as in [31, 32, 124] or considering other battery models that are widely used in the lithium-ion battery community [24].

[1]**Reprinted from [143]: A. V. Vykhodtsev, D. Jang, Q. Wang, W. Rosehart, and H. Zareipour, "Linearized physics-based lithium-ion battery model for power system economic studies". 11th Bulk Power Systems Dynamics and Control Symposium (IREP 2022), 2022.**

The dynamics of the processes inside the lithium-ion battery can be captured if the physics-based models derived using the porous electrode theory [109] are employed. However, most of these models are too complex for the optimization framework because they are formulated using coupled partial differential equations and various nonlinear algebraic expressions. Several authors such as [39] and [38] performed power systems optimization studies with the single particle model, which is the simplest among the physics-based models. The main limitation of their optimization framework is a nonlinear formulation that suffers from convergence problems and does not ensure global extrema. Moreover, the optimal charging/discharging profile presented in [38] did not guarantee constant power output over one hour commitment period for the energy arbitrage. Both authors have not explored the impact of the detailed battery model on the resulting optimal profile in the short term and were mostly focused on the impact of degradation.

In this paper, a linearized physics-based model is introduced to improve accuracy and feasibility of the lithium-ion battery energy storage system operation strategy. Compared with [32] and [36], the proposed model for the battery operation is built using concepts of physics and it is computationally attractive from the optimization framework perspective. Unlike prior works [39] and [102], where a nonlinear optimization framework was built, in this work, a mixed-integer linear programming is formulated that can be solved using commercial off-the-shelf solvers. In contrast to [38], the focus of this work is a short-term operation of LIBESS. The comparison between the proposed model and a simple power-energy model is performed using the energy arbitrage application.

3.2 Methodology

This section first presents a brief overview of the single particle model. More detailed information about this model can be found in [110]. Then a linearized version of equations suitable for a mix-integer linear programming is proposed. The assumptions are discussed and justified. Finally, the energy arbitrage application problem with the proposed lithium-ion battery model is formulated.

3.2.1 Single particle model

The single particle model [110] is the simplest among the analytical models derived from the porous electrode theory [109]. Among physical processes occurring in the lithium-ion cell, this model only includes the transport of lithium within the active material of electrodes and the description of electrode reactions [108]. Limiting the description of a battery to only these phenomena narrows the range of application of the model: it can be used only for low C-rates [110]. However, this is acceptable for energy markets where LIBESS is not employed for high charging and discharging currents.

In the single particle model, the electrodes of the cell are replaced with uniform spherical electrode particles with radii R^i. The superscript i is replaced by p for the positive electrode and it is changed to n for the negative electrode. The transport of lithium inside electrodes is governed by a one-dimensional parabolic partial differential equation in spherical coordinates, as follows [110]:

$$\frac{\partial c^i}{\partial t} = \frac{D^i}{{r^i}^2}\frac{\partial}{\partial r^i}({r^i}^2\frac{\partial c^i}{\partial r^i}), \tag{3.1}$$

where c^i is the concentration of lithium atoms in the electrode particle, r^i stands for a radial coordinate, and D^i is the diffusion coefficient of lithium in the electrode active material. This equation is combined with a set of constraints to conserve symmetry and to include the molar flux of lithium ions J^i as a result of the electrode reactions, as follows [110]:

$$(D^i\frac{\partial c^i}{\partial r^i})_{r^i=0} = 0 \tag{3.2}$$

$$(D^i\frac{\partial c^i}{\partial r^i})_{r^i=R^i} = -J^i. \tag{3.3}$$

The initial condition for the diffusion equation, i.e., the initial concentration of lithium in the electrode, indicates the initial state-of-charge of the lithium-ion cell:

$$(c^i(r^i,t))_{t=0} = c_0^i(r^i), \tag{3.4}$$

where $c_0^i(r^i)$ is the initial concentration of lithium in the electrode.

The Butler-Volmer kinetics equation [112] is employed to characterize electrode reaction. This quantifies the molar flux of lithium ions and it is expressed as:

$$J^i = \frac{2j_0^i}{F}\sinh(\frac{F\eta^i}{2RT}), \tag{3.5}$$

where F is the Faraday constant, R is the gas constant, η^i denotes the activation overpotential, and T is temperature. The exchange current density j_0^i represents the molar flux of lithium ions at the equilibrium state and is given as:

$$j_0^i = k^i\sqrt{(c^{Max,i} - c^{\text{surf},i})c^{\text{surf},i}c^{\text{el}}}, \tag{3.6}$$

where k^i denotes the reaction rate constant, $c^{\text{surf},i}$ stands for the lithium concentration at the surface of the electrode particle, $c^{Max,i}$ is the maximum concentration of lithium atoms in the electrode particle, and c^{el} is the electrolyte concentration, which is assumed constant for the single particle model.

The potential of each electrode, when there no current flowing through the cell, depends on the concentration of lithium on the surface of the electrode, $c^{\text{surf},i}$. This open-circuit potential, OCP^i, is determined experimentally for each type of electrode chemistry. During charging or discharging, the potential of the electrode deviates from the open-circuit potential, and is known as the solid-phase potential, ϕ^i, and is expressed as:

$$\phi^i = \eta^i + OCP^i(c^{\text{surf},i}), \tag{3.7}$$

The applied charging/discharging current is linked with the molar flux of lithium ions through equation (3.8) for the positive electrode and equation (3.9) for the negative electrode respectively, as follows:

$$J^p = -\frac{IR^p}{3\nu^p\varepsilon^p F} \tag{3.8}$$

$$J^n = \frac{IR^n}{3\nu^n\varepsilon^n F}, \tag{3.9}$$

where ε^p and ε^n denote the volume fraction of active material in the corresponding electrode, ν^p and ν^n are volumes of each electrode. The voltage of the lithium-ion cell is expressed as:

$$V_t = \phi^p - \phi^n. \tag{3.10}$$

If LIBESS consists of N identical lithium-ion cells the supplied or consumed power is calculated through applied current and voltage across the cell:

$$P_t = NI_tV_t \tag{3.11}$$

3.2.2 Proposed linearization of the single particle model

The set of equations shown above presents a challenge to be incorporated into the solvable optimization framework that can ensure a quick solution and guarantee optimality. Here, the techniques that can bring the equations and nonlinear expressions to the linear formulations are discussed. The linearized physics-based model will be used to refer to the proposed battery model.

The approximate solution to the diffusion equation with the boundary conditions can be obtained through the combination of the ordinary differential equation. One of these equations describes the evolution of the average concentration $c^{avg,i}$ within the electrode particle and another one couples surface concentration $c^{surf,i}$ with the average concentration [113, 114], as follows:

$$\frac{dc^{avg,i}}{dt} = \frac{-3J^i}{R^i} \tag{3.12}$$

$$c^{surf,i} = c^{avg,i} - \frac{J^i R^i}{5D^i} \tag{3.13}$$

The finite differences are used to convert the ordinary differential equation into the discretized equation, as follows:

$$c_t^{avg,i} = -\frac{3J^i}{R^i}\tau + c_{t-1}^{avg,i}, \tag{3.14}$$

where τ is a time interval between two consecutive measurements of $c^{avg,i}$.

The overpotential η^i can be derived from the Butler-Volmer kinetics equation (2.2):

$$\eta^i = \frac{2RT}{F} sinh^{-1}(\frac{FJ^i}{2j_0^i}) \tag{3.15}$$

The inverse hyperbolic sine in (3.15) can be linearized by using the first term in the Taylor expansion, as follows:

$$\eta^i = \frac{RTJ^i}{j_0^i} \tag{3.16}$$

The equation (3.16) can be further linearized by introducing the piecewise linear approximation for $1/j_0^i$ and then using technique to linearize the product of a binary and a continuous variable. However, to decrease computational cost in this work, it is assumed that the overpotential η^i is not a function of j_0^i and can be expressed as:

$$\eta^i = \frac{RTJ^i}{A^i}, \tag{3.17}$$

where A^i denotes a constant that is selected by the modeller.

The open-circuit potential OCP^i is a nonlinear function of the lithium concentration on

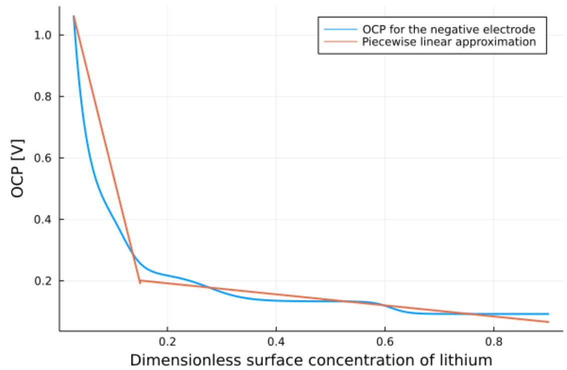


Figure 3.1: The OCP profile for negative electrode made of bi-component Graphite-SiO_x [144] and with its linear approximation.

the surface and should also be modified to reflect the requirements of a mixed-integer linear programming. The piecewise linear approximation depends on the electrode chemistry. In this work, the open-circuit potentials and other parameters for the single particle model are taken from [144]. Figure 3.1 shows open-circuit potential of bi-component Graphite-SiO_x negative electrode with its linear approximation. To include the given approximation into the optimization a binary decision variable is added.

Another bilinear expression that needs to be linearized is the equation for power (3.11). This is done by introducing auxiliary variables y_1 and y_2, as follows:

$$y_1 = \frac{1}{2}(V_t + I_t), \tag{3.18}$$

$$y_2 = \frac{1}{2}(V_t - I_t). \tag{3.19}$$

As result, the right-hand side of the equation (3.11) can be transformed:

$$P_t = y_1^2 - y_2^2. \tag{3.20}$$

The nonlinear terms y_1^2 and y_2^2 are approximated through the piecewise linear technique.

3.2.3 Application of the proposed lithium-ion battery model for energy arbitrage

The optimization problem is the energy arbitrage strategic operation: LIBESS is a price-taker, and no uncertainty is considered. The objective of the LIBESS owner will be to maximize the profit by trading energy over the 24-hour interval. The cost of degradation is included through the energy throughput quantification technique [17]. Two formulations of LIBESS operation, namely the power-energy model and the linearized physics-based model will be compared. The constraints of the optimization problem correspond to the type of LIBESS formulation. The optimal battery operation is defined through (3.21-3.26) for the power-energy model. The charging (ch_t) and discharging (dis_t) powers are decision variables for this model. The energy loss in the power-energy model is considered through a round-trip energy efficiency for the whole cycle η. The state of energy $SoE_{t,r}$ indicates the amount of available energy in LIBESS.

$$\underset{\Xi}{\text{maximize}} \quad \sum_{t=1}^{24} \lambda_t E_t - c_t \tag{3.21}$$

subject to

$$E_t = \sum_{r=1}^{M} \tau(dis_{t,r} - ch_{t,r}) \tag{3.22}$$

$$SoE_{t,r} = SoE_{t,r-1} + \eta * ch_{t,r}\tau - dis_{t,r}\tau \tag{3.23}$$

$$0 \leq ch_{t,r} \leq p^{MaxCh} u_t \tag{3.24}$$

$$0 \leq dis_{t,r} \leq p^{MaxDis}(1 - u_t) \tag{3.25}$$

$$0 \leq SoC_{t,r} \leq Q^{Max} \tag{3.26}$$

where p^{MaxCh}, p^{MaxDis} and Q^{Max} are the charging and discharging maximum power in MW and rated energy capacity in MWh, respectively, λ_t is hourly energy price, E_t stands for energy consumed (negative – for charging operation) or supplied (positive – for discharging operation) within one hour, u_t is a binary variable to avoid simultaneous charging and discharging, τ denotes the duration of time interval r within one hour. The set Ξ contains the state or control variables related to a particular LIBESS model. Auxiliary index r is used to denote time intervals within one hour. The cost of degradation c_t is modelled by:

$$c_t = C_{Q^{Max}} \frac{\sum_{r=1}^{M} \tau dis_{t,r}}{N_{eol}}, \tag{3.27}$$

where $C_{Q^{Max}}$ is lithium-ion battery standalone storage capital cost in \$/MWh and N_{eol} stands for the cycle life of LIBESS.

The optimization framework with the linearized physics-based model is presented by (3.28-3.29). For reasons of space several constraints arising from the discussed linearization approaches are omitted. It is assumed that both models should ensure almost constant power output within one-hour interval participating in electricity trading. Both optimization models are solved with the same time resolution to be consistent in comparison.

$$\begin{aligned} \underset{\Xi}{\text{maximize}} \quad & \sum_{t=1}^{24} \lambda_t E_t - c_t \\ \text{subject to} \quad & (3.4), (3.7) - (3.11), \\ & (3.13), (3.14), (3.17) - (3.20) \end{aligned} \tag{3.28}$$

$$E_t = \sum_{r=1}^{M} \tau P_{t,r} \tag{3.29}$$

3.3 Case Study

In this study, we assume that LIBESS consists of 10,000 LG M50 lithium-ion cells with a nominal energy capacity of 18.20 Wh and a nominal voltage of 3.63 V [145]. The cells are stacked together to form LIBESS with 0.182 MW charging/discharging power and 0.182 MWh nominal energy capacity. The negative electrode of LG M50 cell is made of bi-component Graphite-SiO_x whereas the positive electrode is nickel-manganese-cobalt oxide. The parameters of the lithium-ion cell required for the SPM are taken from [144]. In our model, we limit the charging/discharging current to 1C to be within the limits of the single particle model. The electricity prices for the Alberta electricity market considering estimated carbon prices within the 24-hour interval are shown in Table 3.1. The dimensions of the problem with the power-energy model and the physics-based model are summarized in Table 3.2. Both optimization frameworks were formulated using Julia programming language and they were solved employing Gurobi Optimizer 9.1.2 solver. All simulations were performed on a desktop computer with 48 GB RAM and INTEL i7-8700 CPU at 3.2 GHz. The initial state of LIBESS is fully charged. To limit the number of binary variables in the optimization framework only one linear segment of the negative electrode open-circuit potential was considered. The acceptable range of the negative electrode lithium surface concentration is transformed to state-of-energy $SoC_{t,r}$, the state variable of the power-energy model, using an equation given in [79]:

$$SoC = \frac{c_t^{surf,n} - c^{Max,n}}{c^{Max,n} - c^{Min,n}} Q^{Max} \tag{3.30}$$

The round-trip energy efficiency of the given LIBESS required for the power-energy model was calculated using simulation with the single particle model for 1C current rate, as follows:

$$\eta = \frac{\sum_{r=1}^{M} I_{t=2,r} V_{t=2,r}}{\sum_{r=1}^{M} I_{t=1,r} V_{t=1,r}} \tag{3.31}$$

It was found that $\eta = 0.90$. The round-trip energy efficiency is in fact a function of the current through the cell [84]. This dependence is preserved when the physics-based model is employed. In this work as in most optimization studies with the power-energy model, the round-trip is a constant [30]. The battery capital cost is equal to 567 \$/kWh and is taken from [146] and it is assumed that a given LIBESS reaches the end-of-life criterion after 10,000 full cycles at 1C rate.

Under the power-energy model formulation, LIBESS is operated at the maximum possible charging/discharging power and exploits the two highest arbitrage opportunities between hours 7 and 12 and between hours 19 and 21 (Figure 3.2a). Each time the battery reaches its fully charged state or the lowest state of energy within one hour. The LIBESS operator collects \$39.22 if LIBESS follows this schedule.

Figure 3.2b presents the bidding schedule obtained using the linearized physics-based model. Similar to the strategy obtained with the power-energy model, the bidding strategy of LIBESS is focused on hours with the highest arbitrage. However, LIBESS under this optimization framework does not charge/discharge at the maximum possible charging/discharging power. For example, during hours 12 to 14 when the prices are almost the same it is more beneficial to operate LIBESS at low discharging rates as energy efficiency is higher at these conditions. When the electricity price is significantly higher compared to the adjacent hours such as during hour 2 and hour 21 LIBESS is mostly discharged during this hour. However, the discharging power for these hours is less for the linearized physics-based model as this model does not allow infeasible operations. Both models limit the minimum state of charge and state of energy to the same level of 14%. The resulting profit for the strategy with the physics-based model is 3 % higher than one obtained with the power-energy model and is equal to \$40.72. This is clearly because the power-energy model assumes constant round-trip energy efficiency. If a round-trip energy efficiency was increased to one for the power-energy model the total profit would reach \$41.31.

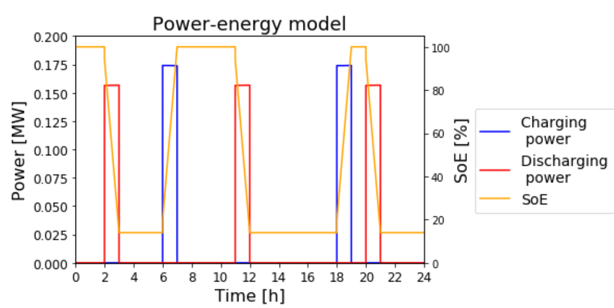
Both LIBESS models are simplifications of the lithium-ion battery. To assess the feasibility of each strategy, the single particle model is simulated with the optimal charging/discharging profile obtained for each model. The percentage of violations during only charging/discharging operation hours is 16% for the power-energy model and 2% for the linearized physics-based model respectively. The optimal schedule obtained using the power-

Table 3.1: The price of electricity.

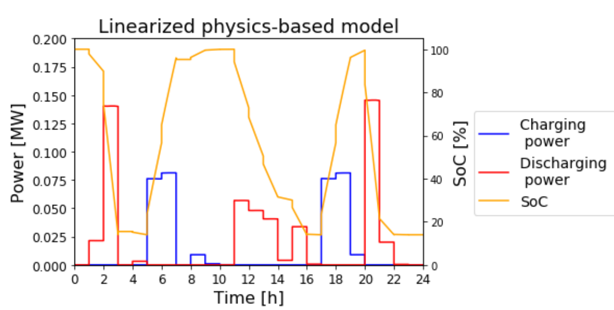
Hour	Price [$/MWh]	Hour	Price [$/MWh]	Hour	Price [$/MWh]
1	132	9	62	17	70
2	170	10	63	18	64
3	175	11	68	19	64
4	133	12	159	20	71
5	135	13	155	21	220
6	62	14	154	22	99
7	56	15	145	23	85
8	63	16	146	24	63

Table 3.2: The dimensions of the optimization framework.

	Power-energy model	Physics-based model
Number of constraints	1272	8688
Number of continuous variables	408	5208
Number of binary variables	24	1464
Time to solve [s]	< 1	27



(a) Power-Energy Model



(b) Linearized physics-based model

Figure 3.2: The charging/discharging schedule calculated using different battery models.

energy model does not guarantee constant charging/discharging power over one hour.

3.4 Conclusion

This paper proposes the linearized physics-based lithium-ion battery model for power system economic studies. The model is built based on the simplifications performed with the single particle model. It was concluded that the proposed lithium-ion battery model provides a more accurate profit estimate and ensures less probability of the execution of infeasible operations compared to the simple power-energy model in the case of energy arbitrage application of LIBESS. In this work, the degradation, a major factor that impacts the profitability of a project with LIBESS, is modelled through a phenomenological model. The advantage of the linearized physics-based model is that it can easily be updated to include the physical description of ageing based on the solid electrolyte interface. The present study has only investigated the proposed model using a simple economic dispatch. The future development of the given work can be done by considering a more complicated market structure or including the system configuration and a network.

Chapter 4

Physics-Aware Degradation Model of Lithium-ion Battery Energy Storage for Techno-Economic Studies in Power Systems[1]

4.1 Introduction

Lithium-ion batteries have already revolutionized the consumer electronics industry, disrupted the transportation sector, and have become a major component of modernizing the electricity grid [148]. The first two applications have one feature in common: the final product should maximize the satisfaction of the user by guaranteeing exceptional performance over the warranty lifespan. In contrast, the justification of lithium-ion battery application in the power grid requires careful cost-benefit analysis as the lifespan of the battery depends on how it is operated. To be a reasonable alternative to conventional grid assets, power system operators should be able to dispatch an energy storage system with a clear understanding of how the requested duty cycle impacts asset degradation and operating costs. Similarly, asset owners must be able to accurately quantify the operating costs for lithium-ion battery energy storage systems in real-time to make strategic decisions that maximize their profitability.

The power systems techno-economic studies with the lithium-ion battery energy storage system (LIBESS) are commonly constructed as an optimization framework that often contains a representation of the the market participation (e.g., energy arbitrage trading [17] or providing transmission services [20]), a model of market interaction of the LIBESS (e.g. a price-taker [22] or a price-maker [18]) and, operational constraints and behavior of the storage system. The latter is usually formulated as a so-called energy reservoir model that may be coupled with the empirical description of degradation [30]. The attraction of these models is that they are simple and linear. However, these models are generally limited in reflecting the true physical performance of the LIBESS, and often rely on limited experimental observations of battery degradation. In the lithium-ion cell community, however, more advanced battery models are employed for simulation purposes for creating a digital twin of battery cells or for the development of battery management systems. Examples of such models are the equivalent-circuit [100] or the physics-based single particle [110] or the physics-based Doyle-Fuller-Newman [149]. A recent review [30] argues that there is a need for more detailed LIBESS models suitable for power system operation and planning studies.

Since LIBESS performance and capacity characteristics degrade with both calendar and operational aging, planning and operation decisions for these assets should carefully consider their unique degradation mechanisms. However, the impact of aging on the operation and the lifetime of a battery is often omitted in power system papers [30]. When degradation of the battery is included into the optimization framework, the following modeling approaches are typically used: direct restrictions on the operational characteristics [41], the energy throughput method [17], the Rainflow or cycle-counting algorithm [42], a linear interpolation of a remaining calendar life [47] and experimentally derived nonlinear formulations [48, 50].

These methods are integrated either into the objective as the cost of the battery degradation [42] or through the additional constraints on the operation [17]. The common feature of these methods is that they rely solely on experience. Only a few modelers such as Reniers [38] and Cao [39] employed the physics-based model, the single particle model, coupled with mathematical formulation of the solid electrolyte interphase (SEI) growth as a degradation mechanism in their optimization framework for power systems. However, the inclusion of these formulations leads to a nonlinear optimization that is difficult to solve over longer planning horizons and their optimality is not guaranteed.

The contribution of this work is the introduction of a new hybrid model of the LIBESS that utilizes linearity of a simple energy reservoir model and follows the rules of physics-based degradation. Unlike previous works [17,42], where the degradation was modeled using an empirical relationship focused on cycling aging, in this work the degradation description is based on the physics of the SEI layer growth. Compared to [48,49,150] where cycling and calendar aging were considered as separate processes, our method is pure physics-based and allows coupling of these degradation processes. The review work [51] was focused on the empirical degradation LIBESS models suitable for use in power system studies. Their estimation of degradation from running the dispatch obtained using the previously discussed models was performed using simulation from nonlinear Rainflow degradation algorithm. However, in this paper, a physics-based validation model incorporating the mathematical description of SEI growth is used. In contrast with [38] and [39], our model is less computationally expensive and global optimality can be specified. The proposed model is based on the energy reservoir concept, and is compared against other models using the energy throughput method and the Rainflow algorithm for degradation estimation. We present simulations for a one-year period in Alberta's 2021 market of the optimal energy arbitrage dispatch of a LIBESS over is used to compare the relative differences between existing and the proposed models. The strategic dispatch was also obtained for various configurations of LIBESS in order to perform a sensitivity analysis of the LIBESS size with respect to the considered battery degradation models. We also present simulation results for the application of the proposed model together with considered empirical models in frequency regulation applications. We have also built an Equivalent Simulation Model to validate the results using an actual single particle model of the lithium-ion cell that includes degradation from SEI growth.

The rest of this paper is organized as follows. The literature review of various LIBESS degradation models used in power system techno-economic studies is presented in Section II. Section III details the mathematical formulation of the single particle model with SEI growth degradation mechanism. This section also presents formulations for the energy reservoir model with the energy throughput and the Rainflow algorithm to describe degradation. In this section, the proposed physics-aware degradation model is formulated. The illustrative case studies are given in Section IV. Finally, limitations and the concluding remarks are provided in Section V and Section VI respectively.

4.2 Background

Modeling the degradation of LIBESS can impact power system operating and planning decisions [30]. In this section, the approaches to model degradation of LIBESS found in power systems techno-economic studies are discussed and compared.

The box constraints on state of energy (SoE) were implemented in several optimization problems to derive the optimal charging/discharging schedule [17, 22, 41]. In [17], it was shown that restriction on the available capacity leads to a longer life of the battery and as a result higher probability to be exposed to more profitable energy arbitrage situations. Authors of [41] showed the net revenue from providing grid services and exploiting energy arbitrage has increased because of the extended life of the battery from limiting the available capacity. However, such constraints can prevent full capacity use for a profitable dispatch of the battery during periods of high price differentials. Although it restricts higher SoE, in general, this approach to model degradation does not consider the impact of calendar aging

[17].

According to the energy throughput concept, a lithium-ion battery is only capable of charging and discharging a finite amount of energy over its lifetime. This means that capacity loss is proportional to the amount of energy cycled through the battery over the given operation horizon. The optimization framework can integrate the energy throughput method either through the degradation replacement cost or enforcing limits on the number of full charging/discharging cycles performed daily [44] or annually [45]. Although the energy throughput method can be easily incorporated into the optimization framework because of its inherent linearity, it does not include the dependence of degradation processes on the average state of charge (SoC) [48], depth-of-discharge (DoD), and charging/discharging current [73]. This method also neglects the impact of calendar aging [17].

The Rainflow algorithm and its several modifications have been widely used in various works to estimate degradation of LIBESS while performing energy arbitrage, providing frequency regulation or peak shaving [42, 47]. The method is an attempt to incorporate the dependence of degradation on the DoD that is missing in the energy throughput concept. The cycle depth stress function is used to assign the amount of degradation from each cycle with the corresponding DoD [42]. This relationship is supported by experimental data, and it is common to indicate at least part of this dependence in the technical specification of the grid-scale LIBESS. The Rainflow technique is used to find the cycles with different DoD in the SoE profile. The corresponding cost of degradation associated with each cycle is calculated from the battery replacement cost of LIBESS [42]. Then this cost is included into the objective function. The Rainflow algorithm is nonlinear by its nature and it can not be formulated in a closed form. Thus, several approaches how to incorporate this method into the optimization framework were suggested. Xu *et al.* [42] introduced a piecewise linear function to approximate the cycle aging mechanism. Kazemi [46] used Benders' decomposition technique to deal with nonlinearity. In [47], a nonlinear optimization solver for a 24-hour optimization horizon was used and the global optimality was guaranteed because of the convexity of the Rainflow method [95]. Albeit, the Rainflow algorithm is a significant improvement compared to the energy throughput method, this approach for the assessment of degradation does not distinguish the average SoC/SoE level near which the LIBESS was cycled. This means that degradation from the 20% DoD cycle around 90% and 40% SOC should be the same which contradicts experimental data of [151]. Moreover, the impact of the discharging/charging rates is also not included. Next, the calendar aging is usually incorporated into the optimization framework through the constant rate of degradation calculated from the battery shelf life [42, 47].

Besides the conventional energy throughput method and the Rainflow algorithm, various nonlinear empirical models were developed and included in the decision-making process in power systems. Maheshwari *et al.* [48] built an empirical degradation model that uses charging/discharging current and SoE dependencies on degradation and employed it for the energy arbitrage application. Their mixed-integer programming problem (MILP) requires a heuristic routine to get a solution. In [49], the degradation cost function based on the DoD and the discharging rate was developed and integrated into a MILP to obtain a bidding strategy in the energy and reserve markets. The optimal biding strategy was determined for a 24-hour interval considering the network constraints of 24 bus system with 10 LIBESS units. Hesse *et al.* [50] derived the strategic operation of LIBESS in the electricity arbitrage application using a degradation model based on the energy throughput and the dependence of the cycle capacity fade on the charging power. This model was incorporated into their MILP solved for one month of operation. The authors did not consider the impact of SoC on degradation and calendar aging was also not included. The impact of calendar aging is also not considered either in [48] or [49]. Authors of [150] included a nonlinear empirical model for cycling and calendar aging based on SoC and DoD and updated the capacity loss in their constraints yearly over the battery lifespan. However, they used only two demand scenarios to represent one year of operation. The nonlinear degradation models described above share the common drawback that they distinguish between degradation contributions from SoC, DoD, and charging/discharging current. However, they result from one dominant degradation process of the solid electrolyte interphase formation. From a computational point of view, Maheshwari [48] and Padmanabhan [49] derived a short-term operation strategy whereas Sayfotdinov [150] considered a longer interval but the author limited the number of demand scenarios to two cases and predefined the hours for the discharge. The calendar and cycling are also presented with separate models as there are no empirical models that coupled them together in these works.

In contrast, the physics-based model such as the single particle model coupled with mathematical formulation of the SEI growth [110] can describe both calendar and cycling aging [52]. The strategic operation of LIBESS for energy and frequency regulation markets was derived using this modeling approach by Reniers in [38] and Cao in [39] respectively. When incorporating this model into the optimization framework, a nonlinear optimization arises. The optimality of the solution for this problem is not assured. Moreover, this framework requires granular resolution of time for the convergence and stability of the problem. For instance, Reniers reported around 6 hours computation time for one week of operation whereas Cao limited the actual optimization horizon to one hour. To solve given problems for a longer period, the model predictive control was used in both studies. The optimality challenge can be addressed by introducing the linearized formulation of the lithium-ion cell as it was developed in [143] for economic energy arbitrage operation of LIBESS over a 24-hour decision-making horizon. However, the solution time increases significantly if the model of SEI formation is added, and longer optimization horizons are considered.

4.3 Methodology

A LIBESS is a complex asset that may consist of thousands of lithium-ion cells, a battery management system, a thermal management system, a fire suppression system, and a power conversion and control system [1]. Compared with the short term-operation of LIBESS where all the components are important in the final model, the aging of LIBESS mostly occurs in the lithium-ion cells. Thus, it is essential to model the degradation of LIBESS from the lithium-ion cell perspective. The proposed model assumes an aggregation approach, where the behavior of a single lithium-ion cell is used to describe the whole LIBESS operation. This modeling approach is considered reasonable if the LIBESS battery management system can maintain relatively uniform cell SoC across the battery array by cell-to-cell balancing techniques. It is also assumed the uniformity of produced cells since a batch or binning process is employed by the manufacturer of the cells [152]. Moreover, this approach to modeling is commonly applied in other studies [52, 150].The impact of temperature is not considered in the proposed model as the thermal management systems of modern LIBESS can generally provide consistently well-controlled and uniform operating temperature for all cells in a given installation [39]. The electrochemical models provide a physics-based description of aging. There are various processes responsible for the deterioration of lithium-ion cell properties. The most significant one is formation of SEI layer [52]. This product of the side reaction is formed on the negative electrode during charging from active lithium and decomposed electrolyte [116]. The aging of LIBESS because of the formation of SEI is a part of the proposed physics-aware degradation model.

In this section, firstly a brief overview is given for the single particle model of the lithium-ion cell; this model is coupled with the description of SEI. The set of equations presented in this subsection is used to construct the Equivalent Simulation Model of LIBESS. This physics-based simulation model is used to accurately estimate and validate degradation effects and is used as the benchmark for comparisons in this paper where it is referred to as "observed degradation." Next, the alternative models used in power system operation and planning studies are given. Finally, the proposed model and underlying assumptions are discussed.

4.3.1 Basics of the single particle model: Equivalent Simulation Model

The porous electrode theory developed by Newman [109] is a base for available physics-based models of a lithium-ion cell. Among these models, the single particle model derived assuming low charging/discharging currents presents a computationally reasonable choice for LIBESS participating in the economic energy arbitrage. This model only describes the movement of lithium in the active material of the electrode, the intercalation/deintercalation reactions, and the thermodynamics of a cell [110]. Uniform spherical electrode particles with radii R^i are used to describe each electrode of the cell. The superscript i is converted to p for the positive electrode and it is replaced by n for the negative electrode. The diffusion equation is used to describe the transport of lithium in these particles, as follows [110]:

$$\frac{\partial c^i}{\partial t} = \frac{D^i}{{r^i}^2} \frac{\partial}{\partial r^i} ({r^i}^2 \frac{\partial c^i}{\partial r^i}) \tag{4.1}$$

where, c^i is the concentration of lithium atoms in the electrode particle, r^i stands for a radial coordinate, and D^i is the diffusion coefficient of lithium in the electrode active material. The boundary conditions for this parabolic partial differential equation contain an equation at the center of the particle to maintain conditions of symmetry and an equation for the molar flux of lithium ions J^i, as follows [110]:

$$(D^i \frac{\partial c^i}{\partial r^i})_{r^i=0} = 0 \tag{4.2}$$

$$(D^i \frac{\partial c^i}{\partial r^i})_{r^i=R^i} = -J^i. \tag{4.3}$$

The initial concentration of lithium in the electrode corresponding to the initial SoC is given as:

$$(c^i(r^i, t))_{t=0} = c_0^i(r^i) \tag{4.4}$$

where, $c_0^i(r^i)$ is the initial concentration of lithium in the electrode.

The variable of the macroscopic description, current, is linked with the variable of the microscopic description, the flux of lithium ions, through equations (4.5) and (4.6) for the positive and negative electrodes respectively, as follows:

$$J^p = -\frac{IR^p}{3\nu^p \varepsilon^p F} \tag{4.5}$$

$$J^n = \frac{IR^n}{3\nu^n \varepsilon^n F} - j^{sei}/F \tag{4.6}$$

where, ε^p and ε^n denote the volume fraction of active material in the corresponding electrode, ν^p and ν^n are volumes of each electrode. Here, j^{sei} corresponds to the current density of the SEI side reaction. This reaction decreases lithium ion inventory and as a result decreases actual energy capacity.

The Butler-Volmer kinetics equation [112] is used to describe the electrochemical reaction on the electrode surface and it is expressed as:

$$J^i = \frac{2j_0^i}{F} \sinh(\frac{F\eta^i}{2RT}) \tag{4.7}$$

where, F is the Faraday constant, R is the gas constant, η^i denotes the activation overpotential, and T is temperature. The exchange current density j_0^i defines the molar flux of lithium ions at the equilibrium state and is given as:

$$j_0^i = k^i \sqrt{(c^{Max,i} - c^{\text{surf},i})c^{\text{surf},i}c^{\text{el}}} \tag{4.8}$$

where, k^i denotes the reaction rate constant, $c^{\text{surf},i}$ stands for the lithium concentration at the surface of the electrode particle, $c^{Max,i}$ is the maximum concentration of lithium atoms in the electrode particle, and c^{el} is the electrolyte concentration, which is constant for the single particle model.

The potential of each electrode, when there is no current flowing through the cell, is called open-circuit potential, OCP^i. This potential is determined experimentally for each type of electrode chemistry. This potential depends on the dimensionless concentration of lithium on the surface of the electrode, θ^i, which is defined as:

$$\theta^i = \frac{c^{\text{surf},i}}{c^{Max,i}} \tag{4.9}$$

During charging or discharging, the potential of the electrode deviates from the open-circuit potential, and is known as the solid-phase potential, ϕ^i, and is expressed as:

$$\phi^p = \eta^p + OCP^p(\theta^p), \tag{4.10}$$

$$\phi^n = \eta^n + OCP^n(\theta^n) + \frac{IR^n}{3\nu^n\varepsilon^n} R^{sei}\delta^{sei}. \tag{4.11}$$

where, R^{sei} stands for the resistivity of SEI layer whereas δ^{sei} is the thickness.

The following equation is used to define the voltage of the lithium-ion cell:

$$V = \phi^p - \phi^n. \tag{4.12}$$

In this study, the SEI mathematical model was based on the formulation suggested in [153, 154]. The reaction of ethylene carbonate with lithium ions leads to formation of SEI. The rate of the side reaction responsible for the formation of SEI follows the Tafel equation and is given as:

$$J^{\text{sei}} = -Fk^{sei}C^{ES,s}\exp\left(\frac{\alpha^{sei}F}{RT}\eta^{\text{sei}}\right) \tag{4.13}$$

where, k^{sei} stands for the kinetic rate constant for the side reaction, $C^{ES,s}$ denotes the concentration of ethylene carbonate on the surface of the negative electrode, α^{sei} is the SEI charge transfer coefficient, and η^{sei} is the overpotential of the side reaction and it is expressed as:

$$\eta^{\text{sei}} = \phi^n - \frac{IR^n}{3\nu^n\varepsilon^n} R^{sei}\delta^{sei} \tag{4.14}$$

The concentration of ethylene carbonate on the surface of the negative electrode is given as [154]:

$$-D^{EC}\frac{C^{ES,s}-C^{ES,0}}{\delta^{sei}}=\frac{j^{sei}}{F} \tag{4.15}$$

where, D^{EC} stands for the diffusivity of ethylene carbonate, $C^{ES,0}$ denotes the concentration of ethylene carbonate in electrolyte.

The rate of SEI layer growth is proportional to the rate of the side reaction [117] and is given as:

$$\frac{d\delta^{\text{sei}}(t)}{dt}=-\frac{J^{\text{sei}}M}{\rho} \tag{4.16}$$

where, M denotes the molar mass of SEI, ρ is the density of SEI. Finally, the loss in the lithium inventory in Ah due to the SEI formation during charging can be estimated as:

$$C_{loss}=-\int_{t_1}^{t_2}\frac{3\varepsilon^p\nu^n J^{\text{sei}}}{3600R^n}dt \tag{4.17}$$

where, $[t_1,t_2]$ is the time interval during which the cell was charging.

The Equivalent Simulation Model of LIBESS used in this work is based on equations (4.1)-(4.17) and is built in the Julia language environment. This model is employed to verify and contrast the results obtained from the optimization. The single particle model employed in constructing the Equivalent Simulation Model was experimentally verified by the lithium-ion cell research community [153, 154].

4.3.2 Baseline model: No Degradation Model

No Degradation Model presents a simple energy reservoir model without battery degradation. The core of this model and all other models used in this work is equation (4.18) which describes a change in the state of energy, $SoE_{d,t}$, during the LIBESS operation. The dispatch of LIBESS consists of commands to charge $ch_{d,t}$ or discharge $dis_{d,t}$ during a given hour. Binary variable $u_{d,t}$ is used to avoid simultaneous charging and discharging. The energy losses in the battery is defined through a round-trip energy efficiency η for the whole cycle as it is commonly used in power system economics studies [24]. The time step Δt is equal to one hour. The following equations/inequalities are used to mathematically define this model:

$$SoE_{d,t} = SoE_{d,t-1} + (\eta ch_{d,t} - dis_{d,t})\Delta t / E^{Nom}, \tag{4.18}$$

$$0 \leq ch_{d,t} \leq p^{MaxCh} u_{d,t}, \tag{4.19}$$

$$0 \leq dis_{d,t} \leq p^{MaxDis}(1 - u_{d,t}), \tag{4.20}$$

$$SoE^{Min} \leq SoE_{d,t} \leq SoE^{Max}, \tag{4.21}$$

$$SoE_{d,t=1} = SoE^{Edge}, \tag{4.22}$$

$$SoE^{Edge} \leq SoE_{d,t=24}, \tag{4.23}$$

$$C_d^D = 0 \tag{4.24}$$

where, p^{MaxCh} and p^{MaxDis} are the charging and discharging maximum power in MW, and SoE^{Min} and SoE^{Max} are the SoE operational limits in MWh. The optimization sub-horizon is limited to 24 hours and SoE^{Edge} is used to link neighboring daily dispatches. The cost of lithium-ion battery degradation C_d^D from one day of operation is presented in (4.24). The indexes d and t are time indexes corresponding to day and hour over one year of operation.

4.3.3 Alternative model: Energy Throughput Model

This model couples the energy reservoir model with the energy throughput method and is similar to one suggested in [17]:

Equations (4.18) – (4.23),

$$C_d^D = c_{LIBESS} \frac{\sum_{t=1}^{24} \Delta t dis_{d,t}}{N_{EoL} DoD^{EOL}} (1 - E_{EoL}) \tag{4.25}$$

where, c_{LIBESS} is LIBESS capital cost in \$/MWh and N_{eol} stands for the total number of cycles at DoD^{EOL} DoD till the battery reaches the end of the operational life. When the battery loses E_{EoL} of the rated energy capacity it should be decommissioned.

4.3.4 Alternative model: Rainflow Model

This model combines the energy reservoir model with an approximation of the Rainflow algorithm proposed in [155]. Here, charging and discharging powers,$ch_{d,t}$ and $dis_{d,t}$, are expressed as segmented variables,$ch_{d,t,j}$ and $dis_{d,t,j}$, with J segments. These equations are similar to (4.18)-(4.23) and they are not given here. The final model is formulated through the following expressions:

$$\text{Equations } (4.18) - (4.23),$$

$$\begin{aligned} C_d^D = {} & c_{LIBESS}(1 - E_{EoL}) J \cdot \\ & \cdot \sum_{t=1}^{24} \sum_{j=1}^{J} \Delta t dis_{d,t,j} \left(\Phi(\frac{j}{J}) - \Phi(\frac{j-1}{J}) \right) \end{aligned} \tag{4.26}$$

where, Φ is a cycle depth stress function that describes the amount of degradation corresponding to a given DoD cycle.

4.3.5 Proposed model: Physics-Aware Model

The control variable for the single particle model is current through the cell and the output is voltage. Both variables are not common variables of the techno-economic analysis where charging and discharging powers are used to characterize the dispatch of LIBESS and SoE is a state variable. Power calculated as a product of two continuous variables, voltage and current, presents a computational challenge if it is integrated into the optimization framework. To convert it to MILP, the difference of squares can be employed as in [143] or using the McCormick envelopes implemented in the Gurobi solver. Both methods require finer time resolutions and a large number of binary variables which is problematic for longer operation horizons.

The proposed solution to this challenge is combining the single particle model with a simple energy reservoir model assuming the identity of all cells, as follows:

$$I_{d,t} = \frac{10^6}{N}(dis_{d,t} - ch_{d,t})/V_{nom} \tag{4.27}$$

where, $I_{d,t}$ is a discretized current though the cell, N denotes the number of identical lithium-ion cells, and V_{nom} stands for the nominal voltage of the cell. In this case the cell voltage is assumed to be constant, and thus, the energy reservoir model is a particular case of the single particle model [19]. However, the real voltage of the cell still can be estimated from the relationship to the input current $I_{d,t}$ and, therefore, can be used to estimate degradation. The following expressions present the hybrid Physics-Aware Model proposed in this work:

$$\text{Equations } (4.18) - (4.23), (4.27)$$

$$J^p_{d,t} = -\frac{I_{d,t}R^p}{3\nu^p\varepsilon^p F} \tag{4.28}$$

$$J^n_{d,t} = \frac{I_{d,t}R^n}{3\nu^n\varepsilon^n F} \tag{4.29}$$

$$c^{avg,i}_{d,t,m} = -\frac{3{J^i}_{d,t}}{R^i}\Delta t_{SPM} + c^{avg,i}_{d,t,m-1} \tag{4.30}$$

$$c^{surf,i}_{d,t,m} = c^{avg,i}_{d,t,m} - \frac{{J^i}_{d,t}R^i}{5D^i} \tag{4.31}$$

$$\theta^i_{d,t,m} = c^{surf,i}_{d,t,m}/c^{Max,i} \tag{4.32}$$

$$OCP^i_{d,t,m} = PWL(\theta^i_{d,t,m}) \tag{4.33}$$

$$\eta^i_{d,t} = \frac{RTJ^i_{d,t}}{j0^i_C} \tag{4.34}$$

$$\phi^i_{d,t,m} = \eta^i_{d,t} + OCP^i_{d,t,m} \tag{4.35}$$

$$\theta^{i,Min} \leq \theta^i_{d,t,m} \leq \theta^{i,Max} \tag{4.36}$$

$$SoC_{d,t,m} = \frac{c^{avg,n}_{d,t,m}/c^{Max,n} - \theta^{n,Min}}{\theta^{n,Max} - \theta^{n,Min}} \tag{4.37}$$

$$SoC_{d,t,m} \geq SoE^{Min}/E^{Nom} \tag{4.38}$$

$$\eta^{sei}_{d,t,m} = \phi^n_{d,t,m} - J^n_{d,t}\delta^{sei}R^{sei} \tag{4.39}$$

$$j^{sei}_{d,t,m} = -Fk_{sei}c_{EC}PWL^{sei}(\eta^{sei}_{d,t,m}) \tag{4.40}$$

$$LLI_{d,t,m} = LLI_{d,t,m-1} - j^{sei}_{d,t,m}\frac{3\nu^n\varepsilon^n F\Delta t_{SPM}}{3600R^n} \tag{4.41}$$

$$C^D_d = c_{LIBESS}LLI_{d_{last},t_{last},m_{last}}V_{nom}\frac{N}{10^6} \tag{4.42}$$

The implementation of the single particle model model either for simulation as the Equivalent Simulation Model or optimization studies as the proposed Physics-Aware Model requires conversion of equations (4.1)-(4.17) into their discrete counterpart. For simulation studies the time step is selected to satisfy the stability condition of the finite difference method for the partial differential equation. In the case of the proposed Physics-Aware Model, the time step was equal to 300 seconds. The decision was made by ensuring that the average difference in voltage obtained from the Equivalent Simulation Model and the proposed Physics-Aware Model was within 5% over the voltage profile.

Equations (4.18)-(4.23) are contribution from a simple energy reservoir model formulation. The linearized formulation of the single particle model is presented in equations (4.28)-(4.38). The equation for the negative electrode flux of lithium ions (4.29) does not have a contribution from the SEI density current since the intercalation current is significantly greater than the current density of the SEI reaction [156]. The one-dimensional diffusion equation (4.1)-(4.4) is converted to the ordinary differential equation using the method presented in [113] and solved using numerical integration (4.30)-(4.31). The expression for the activation overpotential, $\eta^i_{d,t}$, is obtained using the Taylor expansion of (4.7) and setting the exchange current densities,j^i_0, as constants, $j0^i_C$ [157]. The formula (4.36) captures the safety range of the cell operation. The SoC for the hybrid model is defined in (4.37) and this definition is taken from [79]. The expression (4.38) is used to replicate a restriction on SoE for SoC. Equations (4.39)-(4.40) describe the SEI current density. The abbreviation PWL means that the piecewise linearization technique was used for the given expression. Additional insights regarding the linearized formulation of the single particle model and its validation are available in [143].

The integration of SEI description into the optimization framework to maintain a MILP approach requires some simplifications and assumptions. The impact of the SEI layer growth is not considered in the model as the short-term operation is not modeled with the single particle model in this hybrid model. The solid-phase potential ϕ^n (4.35) does not include the contribution from the voltage drop on the SEI layer as it is small compared to other terms. The variation in the concentration of ethylene carbonate on the surface as a result of the mass transfer is also not considered in accordance with the SEI model from [117].

4.4 Case studies

In this section, the results from applying the discussed degradation models are presented for different case studies. First, the strategic behavior of a LIBESS owner derived using these degradation models for electricity prices in Alberta over one year of operation is compared. Then, the size of LIBESS was varied to study the impact on aging while incorporating discussed models in the optimization framework. Finally, degradation models of LIBESS were compared for the frequency regulation application.

4.4.1 Optimal energy arbitrage case study

The four lithium-ion battery models previously described are tested and compared using the economic energy arbitrage use case. The LIBESS owner will trade energy over a one-year period to maximize the profit. The market participation of the LIBESS is a price-taker, and uncertainty in electricity prices is not considered. The electricity prices are electricity pool prices from Alberta in 2021 [158]. The optimization framework for this problem is given as:

$$\begin{aligned} &\sum_{d=1}^{365} \text{Max} \left[\sum_{t=1}^{24} \lambda_t (dis_{d,t} - ch_{d,t}) - C_d^D - c_o dis_{d,t} \right] \\ &\text{Subject to:} \quad \Big\{ \text{LIBESS Model} \Big\} \end{aligned} \tag{4.43}$$

where, the set of constraints {LIBESS Model} represents the set of equations for each of the models discussed before. λ_t is hourly electricity price, and c_o stands for the operational cost of the battery. Without loss of generality, we solve the optimization for each day sequentially over a one-year period. The system level parameters of LIBESS are given in Table 4.1, the cell-level parameters are taken from [144, 159] and parameters for the SEI formulation are drawn from [153,156]. The parameters required to construct the single particle model of this cell are summarized in Table 4.2. Even though the physics-based model is built on the first principles of SEI formation [110] and the model is constructed using a set of experimentally measured parameters, the kinetic rate constant for the SEI reaction was chosen between the values provided in [154] and [156] respectively. Although the system-level parameters (Table 4.1) are assumed they are based on reasonably typical industry values. Selected energy capacity and two-hour duration correspond to a recent trend in higher capacity and duration in the US grids [160].

The modeled LIBESS is constructed from LG M50 lithium-ion cells with a nominal energy capacity of 18.20 Wh and a nominal voltage of 3.63 V [145]. Bi-component Graphite-SiO_x forms the negative electrode, while nickel-manganese-cobalt oxide is used for the positive electrode of the cell. The cells are connected together to form LIBESS with a given energy

Table 4.1: The system level LIBESS parameters.

Parameter	Symbol	Unit	Value
Energy capacity	E^{Nom}	MWh	120
Maximum charging power	p^{MaxCh}	MW	60
Maximum discharging power	p^{MaxDis}	MW	60
Round-trip energy efficiency	η	%	96
Minimum SoE	SoE^{Min}	%	10
Maximum SoE	SoE^{Max}	%	90
Initial and final SoE	SoE^{Edge}	%	10
Battery cycle life: Number of cycles	N_{EoL}	-	2500
Battery cycle life: Specific DoD	DoD^{EOL}	%	100
Battery end of life capacity	E_{EoL}	%	80
Calendar life	T_{cal}	years	20
LIBESS capital cost	c_{LIBESS}	$/MWh	343,000
Operational cost	c_o	$/MWh	5

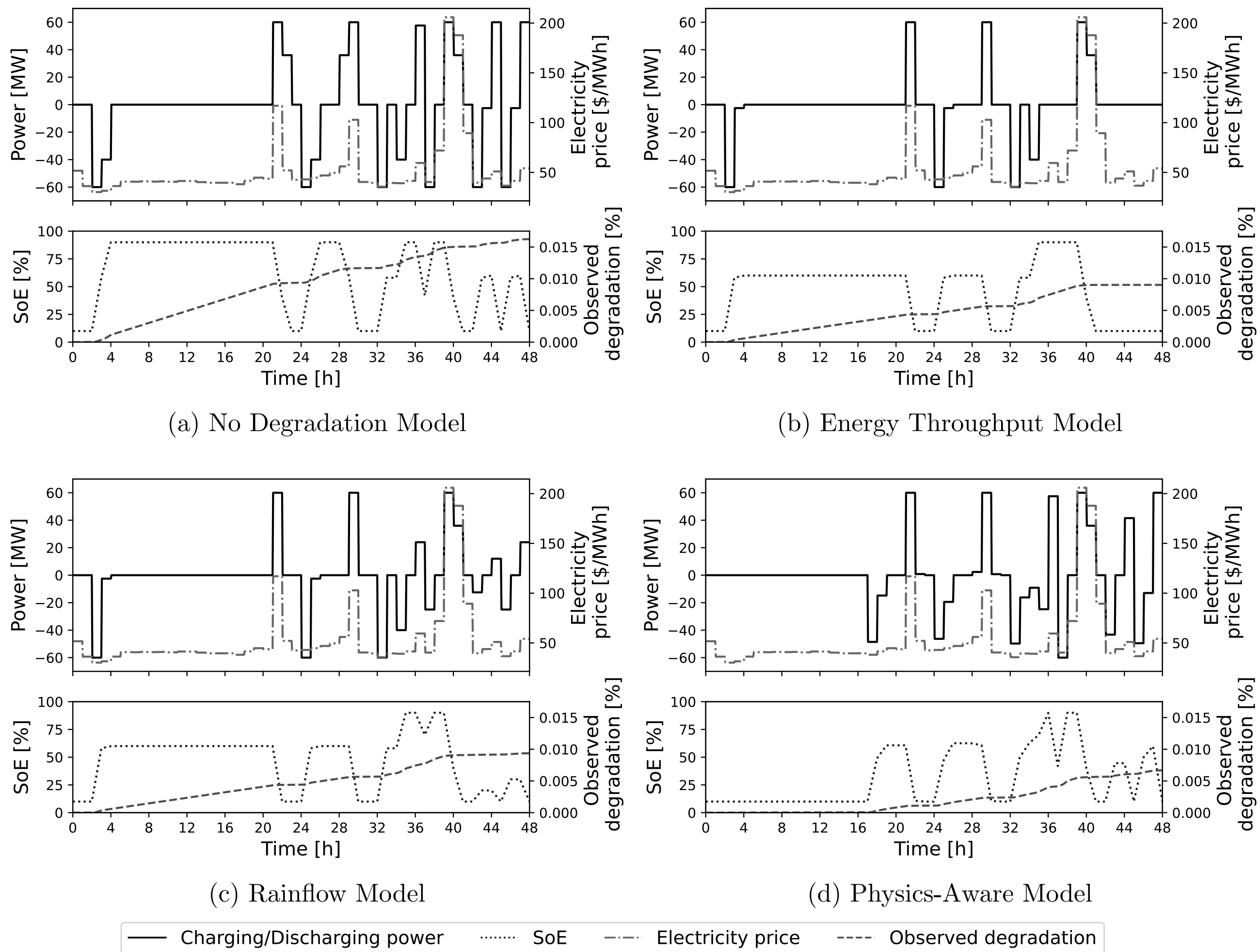
capacity. The degradation characteristics were estimated by running the Equivalent Simulation Model. The cycle depth stress function was adapted from [42] for the Rainflow method. The LIBESS capital cost of 343 $/kWh is taken from [161] where the cost to install the U.S. grid-scale stand-alone LIBESS for durations less than four hours is summarized. The optimization framework was constructed using Julia programming language. The problem was solved using Gurobi Optimizer 9.1.2 solver. All computations were performed on a desktop computer with the following characteristics: 48 GB RAM and INTEL i7-8700 CPU at 3.2 GHz.

Figures 4.1a-4.1d show the differences in operation strategy and observed degradation obtained from the investigated LIBESS models for two arbitrary days. The electricity price signal is given as a reference to understand the trade-off between the cost of degradation and the revenue from energy arbitrage. The charging/discharging dispatch and SoE are given to illustrate their impact on degradation. Each degradation model quantifies degradation differently. Thus, it is reasonable to compare the accumulated or observed degradation using a benchmark as all considered degradation models are approximations of degradation. To this end, and to validate and compare the results, observed degradation is calculated by

Table 4.2: The parameters for the single particle model.

Parameter	Symbol	Unit	Positive electrode	Negative electrode	SEI and electrolyte	Reference
Electrode volume	ν^i	m^3	$7.76 \cdot 10^{-6}$	$8.75 \cdot 10^{-6}$		[144]
Particle radius	R^i	m	$5.22 \cdot 10^{-6}$	$5.86 \cdot 10^{-6}$		[144]
Active material volume fraction	ε^i	-	0.665	0.75		[144]
Diffusion coefficient	D^i	m^2/s	$4 \cdot 10^{-15}$	$3.3 \cdot 10^{-14}$		[159]
Maximum concentration	$c^{Max,i}$	mol/m^3	63104	33133		[159]
(De)intercalation rate constant	k^i	$A/m^2(m^3mol^{-1})^{1.5}$	$3.42 \cdot 10^{-6}$	$6.48 \cdot 10^{-7}$		[144]
Exchange current density	$j0^i_C$	A/m^2	2.7	0.3		[143]
Dimensionless surface lithium concentration at 0% SoC	$\theta^{n,Max}, \theta^{n,Min}$	-	0.9084	0.0279		[144]
Dimensionless surface lithium concentration at 100% SoC	$\theta^{n,Min}, \theta^{n,Max}$	-	0.26614	0.9014		[144]
Electrolyte concentration	c^{el}	mol/m^3			1000	[144]
Kinetic rate constant for SEI reaction	k^{sei}	m/s			10^{-13}	[154, 156]
SEI charge transfer coefficient	α^{sei}	$-$			0.5	[153]
Concentration of ethylene carbonate	$C^{ES,s}$	mol/m^3			4541	[153]
Molar mass of SEI	M	kg/mol			0.162	[153]
Density of SEI	ρ	kg/m^3			1690	[153]
Resistivity of SEI	R^{sei}	$Ohm \cdot m$			$2 \cdot 10^5$	[156]

running the Equivalent Simulation Model with the charging/discharging schedule obtained from solving each optimization problem.



(a) No Degradation Model

(b) Energy Throughput Model

(c) Rainflow Model

(d) Physics-Aware Model

Figure 4.1: The LIBESS dispatch, SoE, observed degradation obtained from the optimization framework using considered LIBESS models and electricity price over two days of operation: 10th and 11th of April, 2021.

Fig. 4.1a reports the dispatch, SoE and observed degradation from the optimization framework with No Degradation Model that maximizes the revenue. As No Degradation Model does not consider degradation, the battery is charged and discharged whenever it makes sense economically. Fig. 4.1a displays a significant growth of degradation from hour 5 to hour 21 since the battery remained at the highest possible SoE. Overall, this model favours higher SoE and maximum available power capacity for charging or discharging.

The dispatch of LIBESS and the associated degradation obtained by using Energy Throughput Model for degradation assessment are shown in Fig. 4.1b. In this case, the dispatch eliminates less profitable cycles which are not able to offset the cost of degradation, e.g. around hour 36. The charging/discharging operation usually occurs at the maximum capacity. Similar to No Degradation Model, this model prefers higher SoE if it is profitable, e.g. around hour 40. The contribution to degradation from hour 5 to hour 21 is less than in the case of No Degradation Model since 60% SoE is chosen from solving the optimization problem. The level of 60% SoE corresponds to only one hour of discharge. This is because only hour 22 generates enough profit to discharge within this hour compared to No Degradation Model with two, at hours 22 and 23.

The Rainflow Model is based on the Rainflow algorithm where the amount of degradation correlates with the level of DoD. The charging/discharging schedule, SoE, and the corresponding degradation predicted with this model are presented in Fig. 4.1c. The dispatch is characterized by a higher number of charging/discharging cycles compared with Energy Throughput Model. In contrast with No Degradation Model, Rainflow Model charges or discharges around lower nominal SoE values to minimize degradation, for example at hours 37, 44, and 48. This is a manifest of the Rainflow algorithm when a shallower DoD is sometimes preferable. Overall, Energy Throughput Model and Rainflow Model predict a similar level of degradation, with the largest contributions correlated to periods with higher SoE.

The dispatch, SoE, and the observed degradation derived with the proposed Physics-Aware Model are reported in Fig. 4.1d. First, the dispatch is more diverse as the charging and discharging powers vary between the cycles. The proposed model favors lower charging powers since the fast charging accelerates the side reaction on the negative electrode [162]. Compared with No Degradation Model, Energy Throughput Model, and Rainflow Model, Physics-Aware Model is mostly operated at lower SoE. This is in line with the experimental studies of degradation as the lifespan of the lithium-ion battery benefits from keeping SoC at lower levels [151]. The degradation from the dispatch obtained using Physics-Aware Model is significantly lower. These observations, the dependence of degradation on the level of power and SoE, are in line with those reported by Reniers with his nonlinear battery model [38]. If Energy Throughput Model and Rainflow Model can include the impact of SoE on degradation in their formulation, their values of observed degradation could be comparable with those from the proposed Physics-Aware Model.

Fig. 4.2 summarizes the revenue in black columns and degradation in grey columns for the whole year of operation for the Energy Throughput Model, the Rainflow Model, and the Physics-Aware Model relatively to No Degradation Model. The degradation-inclusive models do not show a significant change in revenue. There was an approximate 5.2% decline in revenue for Energy Throughput Model, a 4.5% decrease for Rainflow Model, and a 4.3% drop for Physics-Aware Model. Additionally, the absolute values of revenue obtained for each model are as follows: $7,690,949 for the No Degradation Model, $7,287,440 for the Energy Throughput Model, $7,343,406 for the Rainflow Model, and $7,360,127 for the Physics-Aware Model. Although there is no significant change in revenue, the processed energy has decreased by 47.2% for the Energy Throughput Model, by 39.7% for the Rainflow Model, and by 31% for the Physics-Aware Model respectively compared to No Degradation Model. Lower electricity price differentials for these cycles have not significantly contributed to the total revenue in case of No Degradation Model. However, there is a major difference in the observed degradation. Both models B and C predict similar reductions in degradation that are 30% less than the baseline No Degradation Model where it's dispatch does not consider degradation. In contrast, using the proposed Physics-Aware Model, the level of degradation is almost 45% less compared with No Degradation Model.

By extrapolating the findings of this Case Study over a longer period of time and taking into account an end of life threshold of 80% of the LIBESS's initial or nameplate capacity, both the Energy Throughput Model and Rainflow Model predict that the system will reach its end of life after approximately 13 years. However, the Physics-Aware Model ensures an additional 3.7 years of operation beyond that. In this particular case study, this corresponds

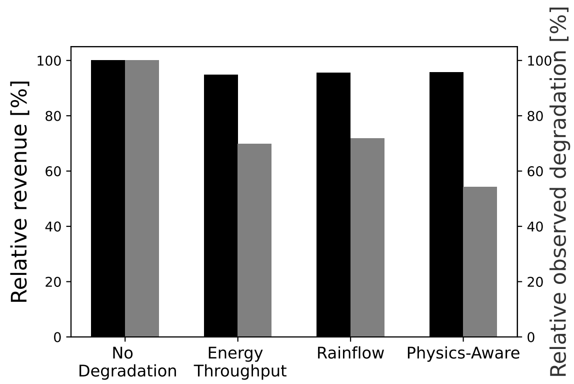


Figure 4.2: Relative to No Degradation Model revenue (left bar) and observed degradation (right bar) of LIBESS over one year of operation using different battery models.

to almost 30% of extra revenue over LIBESS lifespan.

The primary focus of this paper is on degradation modeling of LIBESS, and as such, the proposed modeling approach for all considered models does not take into account losses from the power conversion system. To address the impact of the power conversion system, derived optimal schedules were passed through the power converter efficiency model taken from [163].This model applies the identical formula for power flow in both directions in the study. The analysis revealed that there was no substantial reduction in revenue across the examined models, with the No Degradation Model declining by 3.11%, the Energy Throughput Model decreasing by 2.51%, the Rainflow Model decreasing by 2.76%, and the Physics-Aware Model decreasing by 2.94% respectively.However, both the Rainflow Model and the Physics-Aware Mode showed higher revenue loss compared to the Energy Throughput Model as they have a preference to lower charging/discharging power. In this power range, the power conversion losses are higher.

4.4.2 Sensitivity to the LIBESS size

The previous subsection was focused on the comparison of degradation models for the fixed LIBESS energy capacity and fixed inverter size, i.e. the maximum charging/discharging power. Here, these parameters of LIBESS were varied for the same year of operation. The

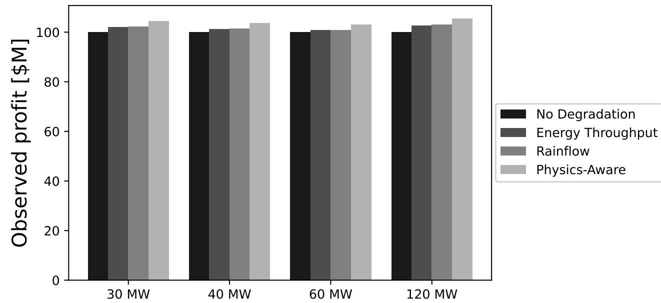


Figure 4.3: Observed profit for different battery models with different inverter sizes.

observed profit and the observed degradation are utilized for the comparison. The observed profit results from the revenue earned from each strategic operation or dispatch schedule, less the associated operating and observed degradation costs. Four sizes of power conversion system from 30 MW to 120 MW for a 120 MWh LIBESS were selected for analysis. The observed profit for one-hour duration storage, i.e. the charging/discharging power capacity is equal to 120 MW, was also corrected as the corresponding dispatch sometimes violates the safety range of the Equivalent Simulation Model [143].

The impact of the maximum charging/discharging power is shown in Fig. 4.3 for the observed profit. The observed profit increases linearly with the maximum rated power for all the models. The observed profit is the largest for the proposed Physics-Aware Model for all considered sizes of inverter. The difference in the observed profit is negligible between Energy Throughput Model and Rainflow Model.

The observed degradation relative to No Degradation Model for the selected power ratings is given in Fig. 4.4. For the reference, the absolute observed degradation for No Degradation Model increased by 20% from 30 MW to 120 MW as higher charging/discharging power and higher SoE contribute more to aging for all the models. The trend of a lower degradation for the proposed Physics-Aware Model is valid for all maximum charging/discharging powers. It is interesting to note that the profile of relative degradation for each inverter size remain almost the same. The reason is that the average SoE for each model does not vary significantly as it is presented in Fig. 4.5.

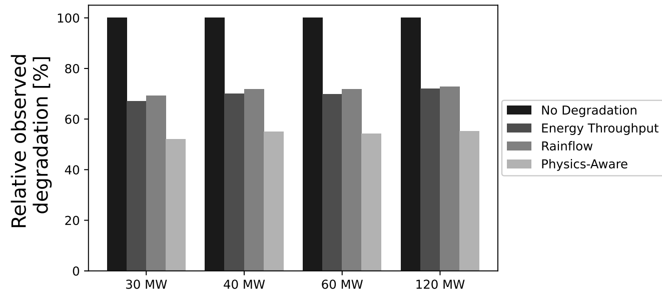


Figure 4.4: Observed relative to No Degradation Model degradation for different battery models with different inverter sizes.

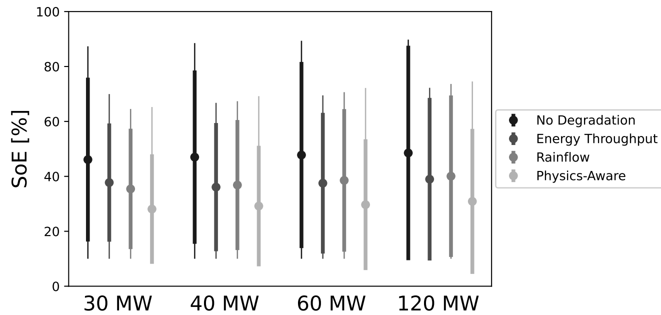


Figure 4.5: Minimum, maximum, standard deviation and mean SoE for LIBESS models with different sizes of the inverter over one year of operation. A thinner line on the plot corresponds to the minimum-maximum scatter, a thicker line corresponds to the standard deviation, and the blob is an average value.

4.4.3 Degradation from the frequency regulation protocol

The proposed degradation model was also tested for the typical frequency regulation dispatch. The standardized US Department of Energy frequency regulation test protocol proposed in [164] was used. This 24-hour duty cycle was repeated consecutively for 365 days. All discussed models were used in simulation mode and compared against the Equivalent Simulation Model. The LIBESS size remained consistent with the economic energy arbitrage studies: 60 MW of power and 120 MWh of energy capacity respectively. As per the test protocol, the frequency regulation duty cycle started with an initial LIBESS SoE of 50%.

The amount of degradation with respect to the total energy capacity was at 5.24% for the Energy Throughput Model, 0.79% for the Rainflow Model, 1.75% for the proposed Physics-

Aware Model, and 2.01% for the Equivalent Simulation Model. The Energy Throughput Model overestimates degradation as it does not differentiate various control modes of operation such as cycles with higher or lower DoD. In contrast, the Rainflow Model considers this impact but omits the impact of SoE and calendar aging in general. The comparison of simulation between the Equivalent Simulation Model, which is a physics-based model without simplifications, and the proposed model helps to evaluate accuracy of this model. The proposed Physics-Aware Model yields results that are more consistent with the Equivalent Simulation Model and those expected from actual cell measurements. The proposed Physics-Aware Model underestimates degradation only by 13%.

4.5 Limitations

Although the proposed Physics-Aware degradation Model provides the modeler with a more accurate estimate of the degradation process, the cost of computation for the optimization problem with this model is higher compared with more popular but less accurate alternatives. Table 4.3 highlights the main characteristics of the corresponding optimization framework. The number of binary variables and constraints used for the proposed Physics-Aware Model is significantly higher. As a result, on average, it takes about 120 seconds to calculate the optimal daily operation schedules with the proposed Physics-Aware Model. This is significantly longer compared to the Energy Throughput Model and Rainflow Model where they generally take less than 30 milliseconds for the same task. Furthermore, for 14 days out of the 365 simulated days, it took significantly longer than average, i.e., about 30 minutes, to solve the optimization with the proposed model. This is due to the mixed integer nature of the optimization and is influenced by the complexity of the daily market price pattern.

It is worth noting that despite the higher computation times compared to existing models, the amount of time required for computing an optimal solution remains reasonable compared to other reported studies where advanced LIBESS models were employed. For example, 2000

Table 4.3: The dimensions of the optimization framework for one day of operation.

	No Degradation	Energy Throughput	Rainflow	Physics-Aware
Number of constraints	265	265	1513	25369
Number of continuous variables	72	72	792	9336
Number of binary variables	24	24	24	2616
Average time to solve [s]	0.014	0.014	0.027	119.713

seconds of computation time and a special temporal decomposition technique was required to obtain a dispatch for one week of operation using a linearized nonlinear degradation model in [48] with GAMS as a programming language and CPLEX as a solver. In [38], the optimization problem for one week of LIBESS operation was built using C++; the IPOPT solver required 6 hours to calculate the solution.

High computational times is generally a modeling limitation when they involve large-scale stochastic power system planning studies over a long simulation horizon. This limitation has driven innovations in three dimensions to mitigate computation burden by: (i) reducing the problem size where possible, (ii) reducing the optimization time horizon by means of time aggregation techniques, and (iii) decomposing the problem and using parallel and high performance computing [165].

4.6 Conclusion

This paper proposed a new LIBESS model that contains electrochemical description of degradation. This model is a hybrid by the formulation as it is built from the system-level and cell-level assumptions, and includes physics-based variables that describe a key degradation process with a lithium-ion cell. The SEI growth was chosen as a main degradation mechanism. The model possesses a valuable property of linearity that makes it suitable for MILP in power system economics. As the proposed mathematical model of LIBESS is an approximation of the real physics-based model, that can be incorporated into the optimization framework, the Equivalent Simulation Model was also constructed to evaluate real degradation from the derived dispatch. The model was benchmarked to two widely used LIBESS battery models with degradation, namely the energy throughput method and the Rainflow algorithm. The proposed model resulted in a lower energy capacity loss whereas it provided the LIBESS owner with almost the same level of the profit. The future development of the given work will include a business case with more market products. The proposed Physics-Aware Model can be also upgraded in future studies to include other degradation mechanisms, such as lithium plating or surface cracking [52].

Chapter 5

AI-Assisted Physics-Based Model of Lithium-ion Battery for Power Systems Operation Research[1]

5.1 Introduction

The lithium-ion battery energy storage system (LIBESS) has been proved as a crucial component of power systems' strategy towards decarbonization, reliability, stability, and resilience [1, 2]. Moreover, the declining cost of lithium-ion batteries allows for their greater adoption by the grid [12]. The monetization of this asset class for investors depends on local regulatory and power market conditions, as well as the strategic commands to the energy management system. There is evidence that the market for ancillary services has become saturated for LIBESS in some progressive jurisdictions [166]. Furthermore, the substantial integration of renewable energy sources into the power grid makes the energy market more volatile, generating interest among investors and physical traders in leveraging LIBESS for economic energy arbitrage. The provision of ancillary services has a mild impact on the

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state of health (SoH) or the percentage of available energy capacity of the battery [142]. In contrast, the operational protocol from energy arbitrage is more damaging to the battery and energy efficiency represents a critical element for a profitable trade. Nonetheless, operational decisions or commands to the energy management system about monetizing LIBESS is usually derived through a simple linear model of LIBESS [30].

This established practice is inconsistent with the complexity of LIBESS, as it is an expensive asset with nonlinear operational characteristics and a limited lifespan that depends on its operational history. This is also supported by a limited number of evidence from field data, where the total energy efficiency and degradation were found to be dependent on LIBESS applications [167]. Therefore, accurately modeling the operational characteristics of LIBESS in the power system decision-making process is crucial. In general, the LIBESS models used in power system operation research can be divided into empirical models, physics-based models, and data-driven models. Only a few works use the latter two models to represent grid-scale battery in techno-economic studies [30].

The empirical models are mostly built around the energy reservoir model, which only tracks the change in the state of energy (SoE) of the battery and assumes constant permissible power and energy efficiency. This model can be enhanced by incorporating certain aspects of lithium-ion cell operation and degradation. This can be achieved by taking into account the relationship between the maximum allowable charging/discharging power and the state of energy, as mentioned in [32, 35]. Another improvement is to consider the impact of the state-of-energy and charging/discharging power on the energy efficiency, as discussed in [31]. It is also possible to combine both dependencies in the battery model, as studied in [33, 71]. In addition to these modifications, a simple energy reservoir model can also be integrated with a degradation description of the battery resulting from cycling or calendar aging. The incorporation of degradation into this model is typically achieved through one of the following approaches: imposing operational limits [44,45], utilizing the energy throughput method [17], or employing the Rainflow algorithm that differentiates the impact from cycles with different depth of discharge (DoD) [42]. Several more advanced empirical-based energy capacity fade formulations, coupled with the energy reservoir model, have been proposed by researchers. Maheshwari [48] considered the impact of charging/discharging current and state of energy, Padmanabhan [49] focused on DoD and discharging rate, while Sayfutdinov [150] incorporated dependencies on state of charge (SoC) and DoD. Overall, these methods share a common characteristic of relying solely on empirical experience. Additionally, while the consideration of calendar and cycling aging is presented separately, it is important to note that both types of aging originate from the same physical process: the growth of the solid electrolyte interphase (SEI) [40].

The physics-based models encompass the description of LIBESS as a physical system. By considering the physical processes occurring within the battery, a more complex relationship between the control and state variables of the LIBESS model can be taken into account. Furthermore, this approach enables the characterization of degradation processes within the lithium-ion cell using fundamental physical laws. Reniers [38] and Cao [39] incorporated the physics-based model, specifically the single particle model, along with a mathematical formulation of SEI growth, as a main degradation process to obtain strategic dispatch of LIBESS participating in electricity arbitrage and providing frequency regulation services, respectively. Both authors built their formulation as a nonlinear optimization problem which is characterized by computational complexity and does not guarantee of achieving optimality. The hybrid model, which combines a simple energy reservoir model with the single particle model, was proposed in [147]. The model offers advantages due to its linear nature and physics-based formulation of degradation. However, it lacks the consideration of the variation in the energy efficiency depending on operational conditions, and the optimization framework does not account for capacity and power fade during long-term studies.

Recently, several data-driven approaches have been proposed in the literature to derive an optimal scheduling of LIBESS in power systems. Zhao *et al.* [62] constructed a neural network to predict degradation by incorporating aging factors such as ambient temperature, charging/discharging rate, SOC, DOD, and current SOH as inputs. The dispatch of LIBESS, placed in a small microgrid with renewable generation plants, was performed iteratively using a standard optimization framework. The framework was updated in each iteration with results obtained from the knowledge generated by the neural network. In the study by Cao [63], a deep reinforcement learning method incorporating operation-dependent energy efficiency and the Rainflow algorithm for degradation assessment was employed for LIBESS participating in the energy arbitrage. Their model-free approach resulted in better revenue estimates compared with traditional model-based optimization methods. The authors of [65] deployed an extreme learning machine to quantify the degradation of LIBESS in their vehicle-to-grid demand peak shaving operation problem. The degradation model, trained using data generated from empirical DOD and charging/discharging rate stress functions, was incorporated into the optimization framework. This was made possible because of the inherent linearity of the extreme learning machine, which does not have any activation functions in its architecture. Overall, the LIBESS aging model they developed yielded an energy capacity loss comparable to that estimated by the Rainflow algorithm, while requiring less computation time. These data-driven LIBESS models proposed above have a common drawback they were constructed using the empirical models and were primarily focused on degradation.

This paper presents a physics-inspired model for a merchant LIBESS facility participating in the real-time energy market. The model incorporates the physics of lithium-ion cell technology to simulate both operation and degradation while being computationally feasible for operation research studies. In contrast to prior studies [17, 42], which utilized an empirical relationship primarily focused on cycling aging to model degradation of LIBESS, our work adopts physical laws for degradation description. Unlike previous works [48, 49, 150], where cycling and calendar aging were treated separately and empirically, our approach is based on the physics of the SEI layer growth. Moreover, our optimization framework includes a physics-based description of varying energy efficiency as well. In contrast with [38] and [39], our model is a mixed-integer linear model making it suitable for power systems techno-economic studies. This work presents an alternative approach to the one proposed in [147]. In contrast to the approach taken in [62], where the neural network responsible for degradation estimation and the optimization framework were heuristically decoupled, our work integrates the neural network within the optimization process and also includes a description of energy efficiency. Compared to [63], where a model-free deep reinforcement learning method with the LIBESS model using varying energy efficiency based on the equivalent circuit model and degradation based on the Rainflow algorithm, our approach follows a traditional operation research method. Unlike the approach used in [65], which employed an extreme learning machine to approximate the LIBESS aging cost function built from DoD and charging/discharging rate assumptions, our model is constructed using feedforward neural networks which preserve the nonlinearity. Moreover, our model takes into account varying energy efficiency and incorporates SEI growth as a degradation mechanism. The inclusion of the physics-based description in our model was achieved through the implementation of the three neural networks that track changes in SoC and SoH and also assess the overall feasibility of operation. The model was validated and compared with the widely-used energy reservoir model.

The rest of this paper is structured as follows. Methodology section provides an overview of the single particle model of the lithium-ion cell, the proposed AI-Assisted LIBESS Model, the benchmark model and, the optimization framework used in the case study. In Section III numerical results for different considerations are presented. The paper concludes with Limitation and Conclusion sections.

5.2 Methodology

The overall goal of this section is to provide a detailed description of the proposed AI-Assisted LIBESS Model. However, first, an overview of the widely-used battery model in power systems techno-economic studies is provided. The term “Baseline Model” is used to refer to this model in this work. This model is used to benchmark the results obtained with the AI-Assisted LIBESS Model. The Baseline Model is an empirical model which is based on the linearity between the SoE and the supplied/consumed power. It also incorporates a linear decrease in the SoH corresponding to the amount of stored energy throughout the battery’s lifetime [17].

The proposed AI-Assisted LIBESS Model is built using the flowchart presented in Fig. 5.1. In Step 1, the Digital Twin of LIBESS is constructed, which can incorporate various lithium-ion battery models commonly used in the lithium-ion cell community [28]. In this work, we utilized the single-particle model with the SEI degradation description [110] to formulate the Digital Twin. In Step 2, the training and validation data points are generated using the Digital Twin. The input part of the dataset consists of the SoH and SoC at the beginning of the operating hour, as well as the consumed/supplied power over this hour. The output part of the dataset provides the SoH and SoC at the end of this operating hour, along with the feasibility classification of this operation. Step 3 is used to construct and train neural networks of the proposed architecture and extract the weight matrices and bias vectors. These neural networks approximate the operation of LIBESS. In step 4, trained neural networks are reformulated with the mixed-integer expressions using the algorithm introduced in [168, 169]. This set of mathematical expressions is referred to as the AI-Assisted LIBESS Model. Finally, in step 5, the proposed model is incorporated into the desired mixed-integer programming formulation.

5.2.1 Baseline Model

The dispatch, SoH, and revenue obtained with the proposed model in this work are compared to those calculated with the Baseline Model. This Baseline Model (5.1)-(5.7) integrates the energy reservoir model to characterize the change in state of energy of LIBESS (5.1) and assessment of degradation through the energy throughput degradation quantification tech-

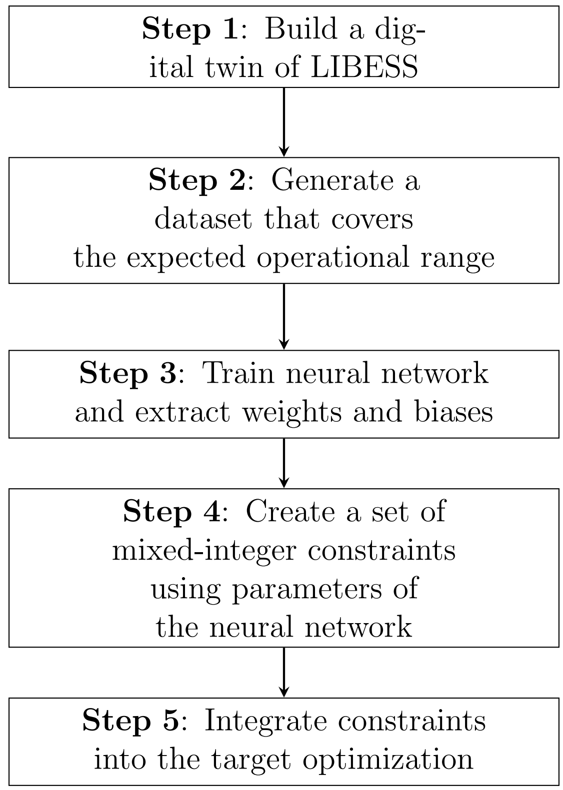


Figure 5.1: Flowchart of the proposed methodology for building AI-assisted LIBESS Model.

nique (5.7) [17]. The operation of LIBESS with the rated energy capacity, E^{Nom}, involves charging ($Ch_{d,t}$) or discharging ($Dis_{d,t}$) commands during a specific hour decided by the optimizer,where d and t are time indexes corresponding to the day and hour over one year of operation, respectively. To prevent simultaneous charging and discharging, a binary variable ($u_{d,t}$) is utilized. The round-trip energy efficiency (η) is employed to evaluate the energy losses in the battery for the entire cycle, as it is commonly used in techno-economic analysis of power systems [143]. The time step Δt is equal to one hour. Here, the charging and discharging maximum power are denoted as p^{MaxCh} and p^{MaxDis}, respectively, both in MW. The operational limits of the state of energy, SoE^{Min} and SoE_d^{Max}, are presented in MWh. The variable SoE_d^{Max} represents the SoH of the battery and is updated daily (5.8). The optimization sub-horizon is equal to 24 hours, and SoE^{Edge} is utilized to connect adjacent daily dispatches. The cost of degradation for a lithium-ion battery during one day of operation, denoted by C_d^D, is determined by equation (5.7). The equation takes into account the capital cost of LIBESS (C_{LIBESS}) in \$/MWh, as well as the total number of cycles (N_{eol}) the battery will undergo at a specific depth of discharge (DoD^{EoL}) until the available energy capacity reaches the end of its operational life, E_{EoL}. The strategic operation is derived on a daily basis until the battery can be decommissioned, and after each day, the maximum available energy capacity is adjusted, as shown in equation (5.8).

$$SoE_{d,t} = SoE_{d,t-1} + (\eta Ch_{d,t} - Dis_{d,t})\Delta t / E^{Nom} \tag{5.1}$$

$$0 \leq Ch_{d,t} \leq p^{MaxCh} u_{d,t} \tag{5.2}$$

$$0 \leq Dis_{d,t} \leq p^{MaxDis}(1 - u_{d,t}) \tag{5.3}$$

$$SoE^{Min} \leq SoE_{d,t} \leq SoE_d^{Max} \tag{5.4}$$

$$SoE_{d,t=1} = SoE^{Edge} \tag{5.5}$$

$$SoE^{Edge} \leq SoE_{d,t=24} \tag{5.6}$$

$$C_d^D = C_{LIBESS} \frac{\sum_{t=1}^{24} \Delta t Ch_{d,t}}{N_{EoL} DoD^{EoL}} \tag{5.7}$$

$$SoE_d^{Max} = SoE_{d-1}^{Max} - \frac{\sum_{t=1}^{24} \Delta t Ch_{d,t}}{N_{EoL} DoD^{EoL} E^{Nom}}(1 - E_{EoL}) \tag{5.8}$$

5.2.2 Digital Twin

The battery Digital Twin is used in this work to generate training and validation datasets for the AI-Assisted Model and as the validation model. The Digital Twin includes the single particle model and degradation description by means of SEI reaction. These formulations have been experimentally validated and implemented in the lithium-ion cell research community [153, 154]. This model is one of the macroscopic physics-based models of lithium-ion cells that is based on the theory of porous electrodes developed by Newman [109]. The governing equations of the model describe the transport of lithium within the electrode's active material, along with intercalation/deintercalation reactions, and the thermodynamics of the cell [110]. The movement of lithium ions between electrodes in electrolyte is neglected. As a result, the model accurately describes the cell behaviour only for low charging and discharging rates that align with the requirements of typical power system applications. Each electrode is represented as a single spherical particle with radius R^i, where i is replaced by p for the positive electrode and by n for the negative electrode respectively. The transport of lithium ions in the model is limited to the active material electrode and follows the diffusion equation [110]:

$$\frac{\partial c^i}{\partial t} = \frac{D^i}{{r^i}^2}\frac{\partial}{\partial r^i}({r^i}^2\frac{\partial c^i}{\partial r^i}) \tag{5.9}$$

where, c^i stands the concentration of lithium atoms in the electrode particle, r^i is a radial coordinate, and D^i denotes the diffusion coefficient of lithium in the electrode active material. The boundary conditions for this partial differential equation maintain symmetry of the electrode (5.10) and describe the molar flux of lithium ions, J^i, at the surface (5.11) [110]. The initial conditions or initial concentration of lithium ion in positive and negative electrodes, $c_0^i(r^i)$, are equivalent to the initial SoC (5.12).

$$(D^i\frac{\partial c^i}{\partial r^i})_{r^i=0} = 0 \tag{5.10}$$

$$(D^i\frac{\partial c^i}{\partial r^i})_{r^i=R^i} = -J^i. \tag{5.11}$$

$$(c^i(r^i,t))_{t=0} = c_0^i(r^i) \tag{5.12}$$

Equations (5.13) and (5.14) establish a relationship between the current and the flux of lithium ions at the electrode's surface, for the positive and negative electrodes respectively. Here, the parameters ε^p and ε^n represent the proportion of active material within the respective electrodes, while ν^p and ν^n denote their volumes. The term j^{sei} is the SEI side reaction current density, which decreases the amount of available lithium ions and consequently lowers the actual energy capacity.

$$J^p = -\frac{IR^p}{3\nu^p\varepsilon^p F} \tag{5.13}$$

$$J^n = \frac{IR^n}{3\nu^n\varepsilon^n F} - j^{sei}/F \tag{5.14}$$

The Butler-Volmer kinetics equation [112] presented in (5.15) describes the electrochemical reaction occurring on the electrode surface. This equation includes the Faraday constant, F, the gas constant R, temperature T, and the activation overpotential, η^i. The molar flux of lithium ions at equilibrium state, i.e., there is no applied current through the cell, is defined by the exchange current, j_0^i, in (5.16). In this equation, k^i represents the reaction rate constant, $c^{\mathrm{surf},i}$ refers to the lithium concentration at the surface of the electrode particle, $c^{Max,i}$ denotes the maximum concentration of lithium atoms in the electrode particle, and c^{el} stands for the electrolyte concentration. It is assumed that this concentration is constant for the single particle model.

$$J^i = \frac{2j_0^i}{F}\sinh\left(\frac{F\eta^i}{2RT}\right) \tag{5.15}$$

$$j_0^i = k^i\sqrt{(c^{Max,i} - c^{\mathrm{surf},i})c^{\mathrm{surf},i}c^{\mathrm{el}}} \tag{5.16}$$

The open-circuit potential, OCP^i, refers to the potential of an electrode if the current does not flow through the cell. This potential is linked to the electrochemical reactions at the electrolyte-electrode interface. It is defined by the electrode chemistry and depends on the electrode stoichiometry or the dimensionless concentration of lithium ions on the electrode surface, θ^i, which is defined in (5.17). In the process of charging or discharging, the electrode's potential differs by the activation overpotential from the open-circuit potential and it is referred to as the solid-phase potential, ϕ^i. The equation (5.19) for solid-phase potential of the negative electrode also reflects the impact of the SEI side reaction.The equation involves two parameters required for the SEI description: R^{sei} represents the resistivity of the SEI layer, while δ^{sei} stands for its thickness.

$$\theta^i = \frac{c^{\mathrm{surf},i}}{c^{Max,i}} \tag{5.17}$$

$$\phi^p = \eta^p + OCP^p(\theta^p), \tag{5.18}$$

$$\phi^n = \eta^n + OCP^n(\theta^n) + \frac{IR^n}{3\nu^n\varepsilon^n} R^{sei}\delta^{sei}. \tag{5.19}$$

The deterioration of the lithium-ion cell capacity and power performance is modeled through the growth of the SEI layer. The SEI mathematical model utilized in this work was taken from [153, 154]. The SEI is formed as a result of the reaction between lithium ions and ethylene carbonate at the electrode surface. The formation of SEI is governed by the Tafel equation (5.20), with k^{sei} representing the kinetic rate constant for the side reaction, $C^{ES,s}$ referring to the concentration of ethylene carbonate present on the negative electrode surface, α^{sei} representing the SEI charge transfer coefficient, and η^{sei} (5.21) indicating the overpotential of the SEI reaction. The concentration of ethylene carbonate on the surface of the negative electrode follows (5.22) [154]. Here, D^{EC} represents the diffusivity of ethylene carbonate and $C^{ES,0}$ denotes the concentration of ethylene carbonate in the electrolyte. According to Ramadass *et al.* (2004), the growth rate of SEI layer is directly proportional to the rate of the SEI reaction (5.23). The SEI layer is characterized by its molar mass denoted by M and density denoted by ρ. The lithium inventory loss in Ah resulting from SEI formation over a time interval $[t_1, t_2]$ corresponding to the charging process may be computed through the utilization of (5.24).

$$J^{\mathrm{sei}} = -Fk^{sei}C^{ES,s}\exp(\frac{\alpha^{sei}F}{RT}\eta^{\mathrm{sei}}) \tag{5.20}$$

$$\eta^{\mathrm{sei}} = \phi^n - \frac{IR^n}{3\nu^n\varepsilon^n} R^{sei}\delta^{sei} \tag{5.21}$$

$$-D^{EC}\frac{C^{ES,s} - C^{ES,0}}{\delta^{sei}} = \frac{j^{sei}}{F} \tag{5.22}$$

$$\frac{d\delta^{\mathrm{sei}}(t)}{dt} = -\frac{J^{\mathrm{sei}}M}{\rho} \tag{5.23}$$

$$C_{loss} = -\int_{t_1}^{t_2} \frac{3\varepsilon^p \nu^n J^{\mathrm{sei}}}{3600R^n} dt \tag{5.24}$$

Finally, the voltage of the lithium-ion cell and the supplied or consumed power by this cell are defined through (5.25) and (5.26).

$$V = \phi^p - \phi^n \tag{5.25}$$

$$P = IV \tag{5.26}$$

In this study, the LIBESS Digital Twin is founded on equations (5.9)-(5.26) and was developed using the Julia programming language. The diffusion equation (5.9-5.12) was solved using the finite difference method.

5.2.3 Proposed AI-Assisted Model

The Digital Twin contains both nonlinear algebraic expressions and partial differential equations that cannot be directly included into the optimization framework with guaranteed optimal solution. In this study, we propose a novel approach to address this issue by replacing the physical equations in the battery model with universal approximators, i.e., neural networks. The proposed AI-Assisted Model replicates the operational characteristics of the battery and can estimate the impact of capacity and power degradation over time. The model is built using a dataset generated with the aid of the Digital Twin. The model calculates the end-of-hour SoC and SoH of the battery within a one-hour period of operation. It considers the consumed or supplied power during the hour, as well as the initial SoC and SoH values.

Structurally, the proposed model consists of three independent feedforward neural networks. Each neural network takes the SoC and SoH at the beginning of the hour, as well as the consumed/supplied power during this hour, as inputs. The output of the first neural network estimates the SoC after one hour of operation based on the input. This network is used to describe the operation of the battery. The second neural network estimates SoH after one hour of operation. This network is used to quantify degradation. This neural network is employed to quantify resulted degradation. Some input data points may lead to infeasible battery operation, a condition not accounted for by either the operation neural network or the degradation neural network. These data points were excluded from the training and validation datasets for both networks in order to eliminate discontinuities in the output. Thus, the third neural network, which is responsible for identifying the infeasible operation of LIBESS, is introduced into the AI-Assisted Model. The training label for this neural network is set at one for infeasible operation and zero for feasible operation. Using three neural networks instead of a single neural network with three outputs has the advantage of eliminating the need for scaling factors when dealing with different outputs.

The proposed architectures of these neural networks are very similar. Each network is composed of an input layer with three neurons, two hidden layers, and an output layer with one neuron. Using a grid search approach for hyperparameter optimization and considering the computational complexity associated with the optimization, we have selected six neurons for all hidden layers of the operational neural network and the degradation neural network, and 12 neurons for the feasibility neural network. The chosen activation function for each neural network is the rectified linear unit, which was selected due to its faster training [170] and compatibility with the optimization framework [168]. The mean absolute error is used as the loss function for both training and validation. Two datasets were created for training and validation, covering operational points of 15 MW/20 MWh LIBESS facility for supplied/consumed power from 0 to 13.6 W, initial SOC from 0.1 to 0.9, and current SoH from 0.8 to 1, with 284,647 and 14,946 data points respectively. Three discussed above neural networks were trained using TensorFlow with Python for 1000 epochs each.

The rectified linear unit produces an output, X_k that equals the input for positive inputs, $\hat{X}_k$, whereas the output is zero for negative inputs (5.27). This expression can be linearized and incorporated into the optimization framework by means of a big M method [169] presented in (5.28)-(5.31). In these equations, the variable k represents the corresponding hidden layer, and l denotes the neuron in this layer. Auxiliary parameters $M_k^{\max,l}$ and $M_k^{\min,l}$ are selected based on (5.32) which should be valid for any possible $\hat{X}_k$. Binary variables y_k^l are also part of this linearization technique.

$$X_k = \max(\hat{X}_k, 0) \tag{5.27}$$

$$X_k^l \geq \hat{X}_k^l \tag{5.28}$$

$$X_k^l \geq 0 \tag{5.29}$$

$$X_k^l \leq \hat{X}_k^l - M_k^{\min,l}(1 - y_k^l) \tag{5.30}$$

$$X_k^l \leq M_k^{\max,l} y_k^l \tag{5.31}$$

$$M_k^{\min,l} \leq \hat{X}_k \leq M_k^{\max,l} \tag{5.32}$$

Equations (5.28)-(5.31) introduce additional binary variables into the optimization framework. In order to reduce the computational burden associated with solving mixed-integer linear programming problem for this framework, some manipulations were made to the neural network parameters, as suggested in [170]. Firstly, certain binary variables were fixed due to their constant status, i.e., the open or closed status of the activation function for any combination of input features. Furthermore, parameters $M_k^{\max,l}$ and $M_k^{\min,l}$ were calculated for a finer range of input features. In contrast to the approach taken in [171], where some matrix weights were enforced to zero during training to create matrix sparsity, we generated extra cuts by analyzing matrix weights.

5.3 Results

5.3.1 Case study

The effectiveness and the performance of the proposed AI-Assisted Model of LIBESS was evaluated and studied using an economic energy arbitrage application. This application allows for the assessment of the inherent faster degradation and impact of energy efficiency on the strategic operation. A merchant LIBESS facility participates in real-time energy market to maximize its profit through energy arbitrage. Price uncertainty is not taken into account to isolate the variations in performance of the modes caused by price forecast errors.

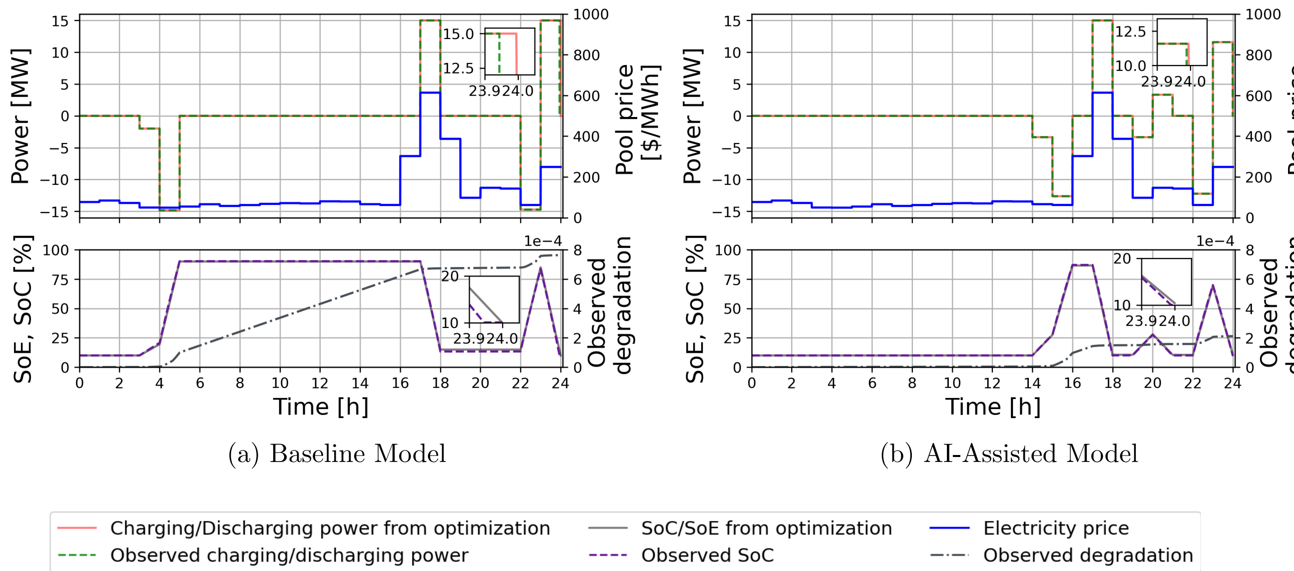
The objective of the optimization framework for the economic energy arbitrage problem is given in (5.33). Here, λ_t denotes the hourly electricity price, N_o stands for the duration of the operation horizon in days, and C_o is the operational cost of the battery. The strategic dispatch was calculated on a daily basis, and the actual amount of degradation was reflected in the subsequent day's operation. This optimization process was repeated every day until the LIBESS reached its end-of-life decommissioning criteria.

$$\sum_{d=1}^{N_o} \text{Max} \left[\sum_{t=1}^{24} \lambda_t (dis_{d,t} - ch_{d,t}) \Delta t - C_d^D - C_o dis_{d,t} \Delta t \right] \tag{5.33}$$

The proposed mixed-integer linear programming framework combining the objective function (5.33) with constraints associated with the corresponding battery model was implemented using algebraic modeling environment JuMP in Julia programming language and solved using Gurobi Optimizer 9.1.2 solver. The computations were executed on a desktop computer that had an INTEL i7-8700 CPU operating at 3.2 GHz and 48 GB of RAM.

Numerical simulation studies were conducted for a LIBESS with a nameplate energy capacity of 20 MWh, a maximum charging and discharging power of 15 MW, and a minimum charging and discharging power of 2 MW. The latter is used to mitigate the power conversion losses at lower power rates [167]. The operating range of SoC was between 10% to 90% as it is defined by manufacturer of the stationary battery storage to prevent under-discharge and over-charge conditions [167]. At the beginning and end of each operating day, the SoC was fixed at 10% assuming intraday utilization of the battery. The energy prices of the Alberta market for 2022 [172] were used to derive monetizing strategy using the proposed Neural Network LIBESS Model and the Baseline Model. These prices were repeated for the subsequent years until the battery reached the end of its operational life, enabling us to track the deterioration of the battery's performance. Moreover, it was assumed that the capital cost of LIBESS is \$156/kWh. This cost is based on an expected decrease of 50% in estimated price of the stationary battery storage in 2021 in the United States [161], along with a probable government tax credit of 30%. The maintenance and operation cost was set at \$2/MWh. Simulated LIBESS is built using LG M50 lithium-ion cells, which have a nominal energy capacity of 18.20 Wh and a nominal voltage of 3.63 V [145]. The negative electrode is made of a bi-component Graphite-SiO_x, while the positive electrode is composed of nickel-manganese-cobalt oxide. These cells are interconnected to create a LIBESS with a specific energy capacity. The parameters for this lithium-ion cell are sourced from [144, 159], while the SEI formulation parameters are extracted from [153, 154, 156].

The comparison between the models and the validation of accuracy are based on the following procedure. The schedule generated from solving the optimization problem with either the proposed AI-Assisted Model or the Baseline Model is used as an input to the Digital Twin. When running the Digital Twin, the input dispatch is adjusted if either the cell voltage or the lithium surface concentration is out of the safety range. This modified dispatch is referred to as corrected dispatch in this work. The revenue or degradation obtained directly from the optimization is called calculated revenue or calculated degradation, while the revenue or degradation obtained from the corrected dispatch is referred to as observed revenue or observed degradation.



(a) Baseline Model

(b) AI-Assisted Model

Figure 5.2: The LIBESS dispatch obtained from optimization and corrected by the Digital Twin, SoE/SoC from optimization and corrected by the Digital Twin, observed degradation obtained from the optimization framework using considered LIBESS models, and electricity price for one operational day: 24th of January, 2022.

5.3.2 Daily strategic dispatch of LIBESS

Before considering the long-term effects of the proposed AI-Assisted Model, this discussion focuses on the operation of LIBESS over a single arbitrary day. Figures 5.2a-5.2b illustrate the variations in the resulted schedule, SoE or SoC, and observed degradation, as obtained from the discussed LIBESS models. Positive power values refer to discharging, and negative values refer to charging of the LIBESS. Analyzing these state and control variables aids in understanding the connection between them, degradation, and energy losses. The operational decisions about the monetization of the battery are determined by the electricity price, which is also provided on the graphs.

Fig. 5.2a shows the dispatch of LIBESS and its degradation using the Baseline Model for degradation assessment and operation. The model selects several of the most attractive price spreads throughout the day. The LIBESS plant charges and discharges at its maximum available power capacity as long as it adheres to the LIBESS nameplate parameters. The dispatch obtained from the optimization was adjusted using the Digital Twin. During the

24th hour, the LIBESS facility was not able to deliver all the committed energy due to the fact that the round-trip energy efficiency remains constant in the Baseline Model. However, the actual efficiency depends on the operating conditions, which are reflected in the Digital Twin. The average daily energy efficiency, calculated from the corrected dispatch, is equal to 92.4%, which is lower than the 95% value used in the Baseline Model. As a result, the battery does not possess sufficient energy to discharge during the last hour. The energy processed, as corrected by the Digital Twin, decreased by 2.76% compared to the results from optimization. With the strategic dispatch, the battery operates at the maximum allowable SoE for most of the day. The SoE plot reveals that the battery reaches a minimum of 10% SoC before the end of the 24th hour. According to the Digital Twin, the most significant contribution to degradation during one hour of operation occurs during the charging periods at hours 5 and 23. However, the overall contribution to degradation is predominantly influenced by operating at the highest possible SoE. In general, the Baseline Model prioritizes higher State of Energy and utilizes the maximum available power capacity for both charging and discharging operations. Following this adjustment with the Digital Twin, the battery plant was able to generate $10,993, which is 1.8% less than the original calculation from optimization. By the end of this operational day, the SoH of the LIBESS reached 99.49%.

The strategic schedule, SoC, and the observed degradation obtained with the proposed AI-Assisted Model are given in Fig. 5.2b. Firstly, there is typically a short time interval between charging and discharging, even though this duration may not align with the most profitable price arbitrage. Secondly, the AI-Assisted Model prioritizes lower charging powers, as the intensity of the SEI formation reaction is weaker under these conditions [162]. The optimizer also determined that the electricity price differential between hours 20 and 21 was sufficient to compensate for the cost of degradation. This contrasts with the schedule result around these hours obtained using the Baseline Model. The energy processed, after being adjusted by the Digital Twin, experienced a 0.85% decrease in comparison to the optimization results. This is lower when compared to the results obtained using the Baseline

Model. The schedule of operation determined using the AI-Assisted Model rests at lower SoC. This is consistent with experimental studies, such as the one conducted by Wikner *et al.* [151], which suggest that maintaining lower SoC levels contributes to a longer lifespan for lithium-ion batteries. The degradation resulting from the dispatch obtained using the AI-Assisted Model is significantly lower compared with one with the the Baseline Model. These findings, highlighting the impact of power level and SoC on degradation, are consistent with those reported by Reniers using a nonlinear battery model [38]. The Digital Twin results in revenue of $10,390 which is 0.9% less compared to estimations with the proposed AI-Assisted Model. The SoH level was at 99.80% at the end of this day. Overall, the results demonstrate that incorporating a physics-based description of LIBESS leads to a more efficient dispatching, resulting in lower degradation, albeit with a 5.5% decrease in revenue.

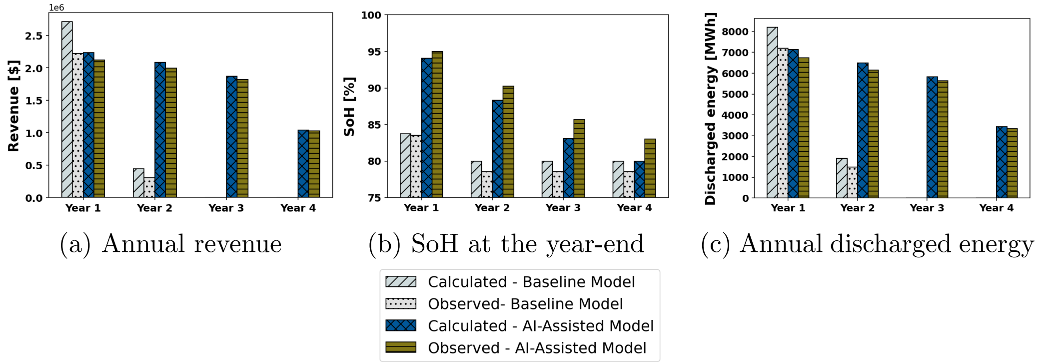
5.3.3 Analysis of long-term performance

The results of the long-term operation of the LIBESS plant using both models for strategic scheduling are presented in this subsection. In this study, the electricity prices observed in 2022 are assumed to remain constant for each consecutive year. The daily optimization process ceased when the battery reached 80% of its SoH estimated as part of the optimization framework.

The distribution of revenue from energy price spread trading with different models over the years, directly from optimization and adjusted by the Digital Twin, is shown in Fig. 5.3a. Both the Baseline Model and the AI-Assisted Model overestimate the revenue from operation. However, the difference in estimated revenue and the observed one is less than 5% for the proposed AI-Assisted Model and more than 18% for the Baseline Model. Moreover, a slight increase in revenue as result of operation with higher degradation in the first year with the Baseline Model leads to the decommission of the battery in the second year. The revenue from strategic scheduling obtained with the AI-Assisted Model declines with years in service, as the performance and available energy capacity deteriorate. The sharp decline in the fourth year is solely attributed to the fact that it operated for only 274 days before reaching the end-of-life criterion.

The evolution of SoH of a LIBESS facility, estimated in optimization and calculated in post processing with the Digital Twin, is presented in Fig. 5.3b. The Baseline Model underestimates degradation, resulting in a decline of more than 15% in SoH in the first year. In contrast, the proposed AI-Assisted Model overestimates degradation and ensures an almost linear decline in SoH over the years. The reason for the mismatch between the estimated SoH from the AI-Assisted Model and the actual SoH calculated with the Digital Twin is the model's lack of accuracy at lower SoC levels. In these lower SoC ranges, where the actual degradation is smaller, the AI-Assisted Model trained with Mean Absolute Error loss function predicts degradation with an error. The degradation with the AI-Assisted Model also exhibits a slight deceleration over the years, decreasing from 5.9% in the first year to 5.2% in the third year. In summary, the deployment of the AI-Assisted Model for dispatch results in the SoH reaching 80% after over three and a half years, while the Baseline Model predicts less than two years of operation in this specific case study.

Fig. 5.3c depicts the annual energy supplied by the LIBESS, considering two strategic dispatches, and the actual energy provided when the resulting schedules are adjusted according to the Digital Twin. For the Baseline Model, the discrepancy between the calculated and observed discharged energy increased from 12.3% in the first year to 22.1% in the second year. This model fails to account for the degradation of battery performance and only tracks the degradation of energy capacity. Additionally, it employs a constant round-trip energy efficiency, unlike the AI-Assisted Model, which incorporates efficiency dependent on operation conditions. The application of the AI-Assisted Model results in a decrease in the difference between the calculated and corrected amount of discharged energy, reducing it from 5.6% in the first year to 2.5% in the final year. This decrease can be attributed to the AI-Assisted Model overestimating the degradation, thereby narrowing the operating range



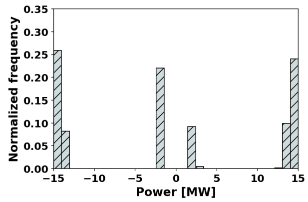
(a) Annual revenue (b) SoH at the year-end (c) Annual discharged energy

Figure 5.3: The annual revenue, discharged energy, and SoH at the year-end of LIBESS providing economic energy arbitrage employing either the Baseline Model or the proposed AI-Assisted Model.

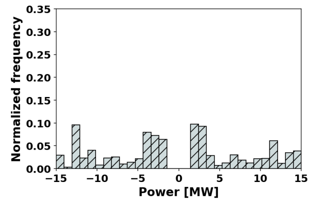
for the LIBESS.

The reason for the rapid degradation of LIBESS, observed when using the simple Baseline Model compared to the AI-Assisted Model, becomes apparent when analyzing the dispatch characteristics over an extended period. For instance, Fig. 5.4a and Fig. 5.4b demonstrate the charging and discharging power distribution during the first year of strategic operation, obtained using the Baseline Model and the AI-Assisted Model, respectively. With the Baseline Model, discrete peaks are noticeable. These peaks represent instances of high charging and discharging power, aimed at exploiting the highest energy price spread, as well as multiple peaks around the minimum power threshold to ensure extreme ranges of SoC. This model does not include the impact of the power on degradation and energy efficiency. In contrast, the distribution of power achieved with the AI-Assisted Model is continuous, as the algorithm selects profitable trades by considering electricity prices, the round-trip energy efficiency and the resulting degradation.

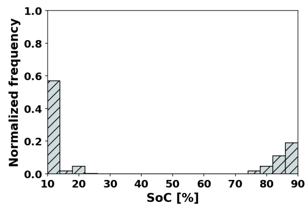
The distributions of SoC for the two considered models over the same one year of operation are given in Fig. 5.4c and Fig. 5.4d. The preferable state for both models is at the minimum empty state of LIBESS, which corresponds to a 10% SoC. However, in order to exploit higher price differentials, the LIBESS often maintains a higher SoC when using the dispatch obtained with the Baseline Model. This is not the case with the AI-Assisted



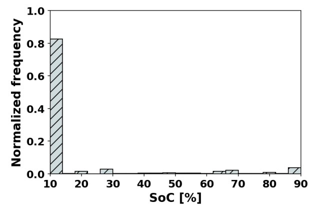
(a) Distribution of power for the Baseline Model



(b) Distribution of power for the AI-Assisted Model



(c) Distribution of SoC for the Baseline Model



(d) Distribution of SoC for the AI-Assisted Model

Figure 5.4: The dispatch characteristics inherent to the Baseline Model and the AI-Assisted Model.

Model, as this model is built from a physics perspective and avoids higher SoC to reduce the contribution of calendar aging [151, 167].

The AI-Assisted Model enables tracking of capacity and power fade, along with the decline in round-trip energy efficiency. Figure 5.5 shows the variation in optimized scheduling for the same day across different years, considering varying SoH of the LIBESS. Firstly, capacity fade leads to a decrease in discharging power at hours 18 and 24 in consecutive years. Secondly, at hours 15 and 16, the charging pattern of the LIBESS facility is modified to ensure compliance within the allowable or safe operating envelope of the battery with the degraded SoH.

5.3.4 Impact of energy efficiency

Previously, the discussion was primarily focused on the the influence of degradation on strategic scheduling. To assess the impact of the round-trip energy efficiency on dispatch, a hybrid model is proposed. This model integrates the Baseline Model with a neural network tasked with identifying infeasible dispatches. In this case, the majority of the mismatch

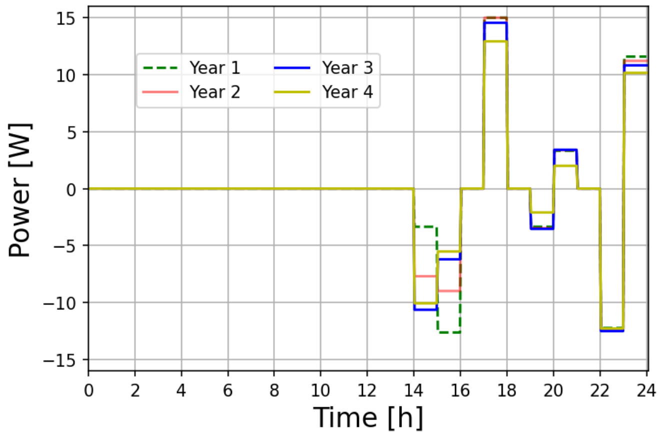


Figure 5.5: The LIBESS dispatch obtained from optimization with the AI-Assisted Model for one operational day repeated for consecutive years.

between the energy discharged as calculated from optimization and the energy observed as a result of correction with the Digital Twin should be primarily due to the assumption of constant energy efficiency in the modeling process. This indirect approach to estimating the role of energy efficiency in the Baseline Model is valid, assuming that the model can accurately monitor changes in SoH, which is one of the input parameters for the neural network to identify infeasible operation of LIBESS. As shown in Fig. 5.3b, there was no significant mismatch between the degradation estimation using the Baseline Model and the one calculated with the Digital Twin. Therefore, our assumption is valid and can be used to estimate the role of energy efficiency in the dispatch calculation.

For the first year of operation, this hybrid model exhibits 10.8% difference between calculated and observed discharged energy, in comparison to 12.3% obtained with the Baseline Model. Consequently, the former difference mostly arises from keeping the round-trip energy efficiency constant. The actual round-trip energy efficiency depends on the operating conditions and declines with aging [97].

5.4 Discussion

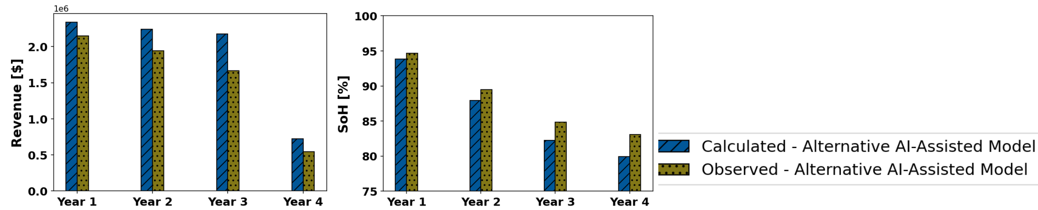
In this section, we will discuss the limitations of the proposed AI-Assisted Model and present an alternative model that is less computationally expensive.

5.4.1 Limitations of AI-Assisted Model

The proposed AI-Assisted Model has several drawbacks. One limitation is that the model is built solely from the perspective of a single component of the LIBESS, namely the lithium-ion cell. In fact, LIBESS is a complex infrastructure comprising five main components: thousands of lithium-ion cells, a battery management system, a thermal management system, a fire suppression system, and a power conversion system [1]. It is reasonable to focus on the degradation assessment of lithium-ion cells when considering a LIBESS, as degradation primarily occurs within this component. However, other components have an impact on energy efficiency and should be considered in future work. In this study, the degradation of power capability and energy capacity is represented by the growth of SEI. However, additional degradation mechanisms can be incorporated, such as lithium plating or surface cracking [52]. The proposed AI-Assisted Model is constructed based on the assumption of a one-hour settlement interval with a fixed charging/discharging power, and it requires retraining if these conditions are changed.

5.4.2 Alternative AI-Assisted Model

The LIBESS facility engaged in energy arbitrage trading should update its bids as a more accurate electricity price forecast become available. However, the proposed AI-Assisted Model does not facilitate fast calculations, especially when using a desktop computer. The average computation time to run daily optimization with the AI-Assisted Model is equal to 1115 seconds. In certain scenarios, generating a solution may require over an hour. This computational challenge can be addressed by combining an energy reservoir model with two



(a) Annual revenue (b) SoH at the year-end

Figure 5.6: The annual revenue and SoH at the year-end of LIBESS providing economic energy arbitrage employing the Alternative AI-Assisted Model.

independent neural networks, one for feasibility and another one for degradation assessment. By adopting this approach, the average running time on the same machine decreased to 14 seconds, with a maximum time of 69 seconds was observed. This is a significant improvement compared to the average of 120 seconds reported in [147], where a constant energy efficiency was also assumed. In this work, the model is referred to as the Alternative AI-Assisted Model.

The improvement in computational time efficiency came at the cost of compromised revenue and SoH estimation accuracy, as illustrated in Fig. 5.6a and Fig. 5.6b, respectively. The average relative difference between the calculated and observed revenue increased to 17% for the Alternative AI-Assisted Model. Nevertheless, the SoH estimation remained consistent with that of the original AI-Assisted Model.

5.5 Conclusion

This paper presents a novel LIBESS model that accurately replicates the battery's operation and is constructed based on the underlying physical system. The incorporation of the physics-based description in our model was performed by using three neural networks that can estimate SoC, SoH, and operational feasibility. The selected architecture allows to incorporate this model into a common mixed-integer linear programming problem in power systems such as one used for energy trading with LIBESS. Overall, this model is able to simulate the degradation of energy capacity and the energy efficiency as function of the operational conditions. The proposed model outperforms the traditional LIBESS model in obtaining the strategic dispatch with higher revenue and prolonged life of LIBESS. The model was also capable of tracking the decrease in energy efficiency and available power over time. As the real-time energy arbitrage trading with an energy storage system requires a fast estimation for a profitable trade, we also proposed the Alternative AI-Assisted Model that compromises some fidelity for major gains in computational speed while maintaining accuracy for SoH estimation.

Chapter 6

Conclusion

This thesis is focused on the development of physics-based models for lithium-ion battery energy storage in power systems' decision-making processes. First, an overview of lithium-ion battery models used in power system operation and planning studies is conducted. Then, a physics-based mixed-integer linear model, based on the single particle model of a lithium-ion cell, is proposed for short-term operation studies. The case study demonstrates that this model enables a more realistic reflection of storage behavior by incorporating fundamental constraints. Next, a model that accounts for physics-based degradation is presented. The long-term performance of LIBESS using this model is compared to calculations based on energy throughput or the Rainflow method. Finally, a data-driven optimization-ready lithium-ion battery energy storage model based on electrochemical formulations is proposed. This model describes power and energy capacity fade, as well as energy efficiency, as a function of the operating conditions. The outcome of this thesis could assist modellers and decision-makers in operating their LIBESS in a more cost-effective manner, while still ensuring safety compliance. The detailed conclusions for each chapter of these thesis are summarized as follows.

Chapter 2 presents the current state of lithium-ion battery modelling in techno-economic studies of power systems and justify the need for further investigation. Firstly, three LIBESS models with varying levels of detail, encompassing both operational characteristics and degradation processes, are reviewed. The governing equations of these models are presented in a suitable format for the optimization framework. Next, a literature review of research papers that derived optimal operation and planning decisions for business cases involving lithium-ion battery storage across various system-level applications is conducted. The reviewed studies are classified based on the LIBESS application, battery model, and employed optimization techniques. Based on the reviewed literature, it can be concluded that advanced battery models can offer more accurate estimates for the economic potential of LIBESS, feasible charging/discharging schedules, and more precise projections of capacity and charging/discharging power fading. Areas for future research associated with lithium-ion battery models in operation and planning problems are also identified.

Chapter 3 introduces the development of a linearized lithium-ion battery model based on fundamental physical laws. The model incorporates various techniques to simplify the set of equations corresponding to the single particle model of the lithium-ion cell. These techniques include the utilization of a parabolic polynomial profile approximation for solid phase diffusion, the adoption of a piecewise linear approximation for physical parameters, the application of Taylor expansion to the Butler-Volmer kinetics equation, and the replacement of a bilinear expression representing the charging/discharging power. The proposed lithium-ion battery model is integrated into the optimization framework, aiming to find a strategic scheduling for the storage owner who wants to participate in economic energy arbitrage over one day of operation. Compared to the traditional energy reservoir model, the schedule calculated with the proposed model results in a lower number of safety violations. This has been verified through a digital twin constructed based on the original single particle model.

Chapter 4 presents a novel mixed-integer linear degradation model for lithium-ion battery energy storage, specifically designed for utilization in power systems operation and planning studies. The model is constructed from the physical aspects of the degradation process. It uses the description of the growth of SEI layer as a main degradation mechanism and a formulation that describes the evolution of SoE based on a typical energy reservoir model. The model is benchmarked against two widely used LIBESS battery models with degradation: the energy throughput method and the Rainflow algorithm. In our case study on energy trading over one year, the proposed model demonstrated a reduction of 45% in energy capacity loss while offering the LIBESS owner with revenue levels that are nearly identical to those calculated using traditional models based on the energy throughput method and the Rainflow algorithm. Moreover, the results indicate an increase in energy capacity loss for all models when the power capability size of LIBESS is increased. The proposed model is also utilized to estimate energy capacity loss for a typical frequency regulation protocol. In comparison to the energy throughput method, which overestimates degradation by 160%, and the Rainflow algorithm, which underestimates it by 60%, the proposed physics-aware model only underestimates degradation by 13%.

Chapter 5 proposes a data-driven, physics-informed model of a LIBESS for the mixed-integer optimization framework. This model accurately captures both the short-term and long-term performance of the LIBESS while preserving the corresponding nonlinearities of the battery system. Three feedforward neural networks, each containing rectified linear activation functions in their architecture, serve as the foundation of this model. These neural networks describe the changes in both the SoC and SoH. By employing this specific choice of architecture, the model can be incorporated into the mixed-integer linear programming as a set of constraints. The model's abilities are demonstrated through the application for economic energy arbitrage using historical prices from the Alberta energy market. First, the advantages of the proposed model compared to the energy throughput reservoir model for a single day of operation are identified. The analysis highlights two key benefits: reduced energy capacity fade and improved feasibility of dispatch. Over a longer period of time, the proposed data-driven model allows for tracking the decrease in energy efficiency and power fade. Moreover, it demonstrates its ability to prolong the lifespan by maintaining lower SoC and avoiding higher charging/discharging power. When the focus is on short-term operations, computational time becomes a crucial factor. In this regard, the proposed model requires some adjustments, as it currently takes an average of 1100 seconds to calculate a daily dispatch with this model. An alternative AI-assisted model is proposed, which focuses only on the degradation aspect, as it is crucial for energy trading with LIBESS.

6.1 Future work

The following list presents potential extensions to the current work:

(a) The proposed models of LIBESS for operation research studies in power systems are built from a single-cell perspective. These models assume that all cell characteristics and their changes throughout the lifespan are the same. Additionally, the models consider the system-level output of the entire system as a scaled output of one cell. Although this approach is valid, as the LIBESS battery management system can maintain a relatively uniform SoC across the battery array through cell-to-cell balancing techniques and the parallel connection architecture of LIBESS [38], the overall energy efficiency and available energy capacity of the system will depend on the cells with the worst performance. Previous studies have explored the impact of variations in degradation characteristics, such as in [173], which utilized actual simulations of thousands of cells with a statistical distribution of cell parameters, and in [174], which considered statistical distributions of cell capacities and degradation levels. However, these studies were focused on simulation modeling and are not suitable for optimization studies. In summary, the proposed LIBESS models could be expanded to incorporate the variability of cell parameters.

(b) The proposed physics-based linearized models from Chapter 4 and Chapter 5 are based on only one degradation mechanism. While the formation of the SEI layer is considered the most significant degradation process [52], future studies can enhance the proposed models by incorporating other degradation mechanisms, such as lithium plating, electrolyte decomposition, or surface cracking [40]. This upgrade becomes particularly important for optimization studies involving second-life electric vehicle batteries in power grid applications, where plating can be considered as a dominant mechanism [175].

(c) Although the proposed approaches for constructing physics-based models can be applied to any lithium-ion chemistry, this study focuses on lithium nickel-manganese-cobalt oxide (NMC) for validation. Specifically, it uses a single type of cell, namely the cylindrical 21700 commercial cell (LG M50). The reason for this choice is the availability of recently measured parameters for this particular cell [144]. However, other chemistries, such as lithium-iron-phosphate (LFP), should also be studied. This is because LFP-based stationary energy storage is expected to dominate the energy storage market by 2030 [176].

(d) The modelling philosophy employed in this thesis only targets the lithium-ion cell as the foundation for all proposed models to characterize LIBESS in techno-economic studies of power systems. However, LIBESS is a complex asset that may consist of thousands of lithium-ion cells, a battery management system, a thermal management system, a fire suppression system, and a power conversion and control system [1]. Although degradation of LIBESS mainly occurs in lithium-ion cells, the short-term performance is highly impacted by other components, such as the power conversion system and thermal management system. Several attempts have been made in the literature to include a description of the power conversion system into the LIBESS model for optimization [19, 50]. However, it should be noted that in these studies, the description of the lithium-ion cell was empirically constructed. The full-scale simulation of stationary lithium-ion storage was conducted in previous studies such as [84, 173, 177]. However, their approaches are not suitable for the optimization environment. In summary, the future model of LIBESS for operation research should include a formulation of other components of LIBESS alongside the lithium-ion cell.

(e) In this work, all the case studies were completed using only a single battery application for the grid, either for economic energy arbitrage or frequency regulation. However, future development of this work will involve expanding the scope to include a business case with multiple market products for revenue stack.

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