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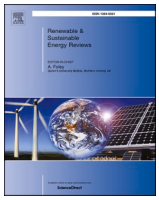

# Lithium-ion battery digitalization: Combining physics-based models and machine learning

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ABSTRACT

Digitalization of lithium-ion batteries can significantly advance the performance improvement of lithium-ion batteries by enabling smarter controlling strategies during operation and reducing risk and expenses in the design and development phase. Accurate physics-based models play a crucial role in the digitalization of lithium-ion batteries by providing an in-depth understanding of the system. Unfortunately, the high accuracy comes at the cost of increased computational cost preventing the employment of these models in real-time applications and for parametric design. Machine learning models have emerged as powerful tools that are increasingly being used in lithium-ion battery studies. Hybrid models can be developed by integrating physics-based models and machine learning algorithms providing high accuracy as well as computational efficiency. Therefore, this paper presents a comprehensive review of the current trends in integration of physics-based models and machine learning algorithms to accelerate the digitalization of lithium-ion batteries. Firstly, the current direction in explicit modeling methods and machine learning algorithms used in battery research are reviewed. Then a thorough investigation of contemporary hybrid models is presented addressing both battery design and development as well as real-time monitoring and control. The objective of this work is to provide details of hybrid methods including the various applications, type of employed models and machine learning algorithms, the architecture of hybrid models, and the outcome of the proposed models. The challenges and research gaps are discussed aiming to provide inspiration for future works in this field.

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## 1. Introduction

To achieve sustainable electrification and decarbonization of the energy sector, reliable energy storage devices are essential. The lithium-ion battery (LIB) is the cornerstone of portable and stationary energy storage in the modern industrial age [1]. It is primarily due to their high specific energy (170–250 Wh/kg), high specific power (200–1000 W/kg), high voltage (3.05–4.2 V), low self-discharge rate (less than 10 % per month), long cycle life (up to 3000 cycles), high efficiency (95 %), high rate capability, low toxicity, safety, compatibility with existing infrastructures and low heat release [2–5]. It is pertinent to note that, despite the exponential growth of LIBs in the last decade, large amounts of electrical energy storage are required to meet societal demands such as growing need for long-range hybrid and electric vehicles [6] and also maintaining reliable electricity supply from renewable energy systems [7]. In addition, more effective controlling strategies, and better battery designs are needed to allow for higher capacity and power, longer lifetime, lower cost, and increased safety [8,9].

It is conventional to develop novel LIB design ideas by testing several prototypes in the lab, which can be costly, unsustainable, and time-consuming [10,11]. Digitalization of LIB development has made it possible to simulate the behavior of a battery in a virtual environment alongside testing actual batteries in the lab [12]. If the simulation method is accurate enough, valuable information about the intricate relationship between the internal battery processes (e.g., ion transport, thermal effects, mechanical stress, and electrochemical reactions) and battery structure and operating condition can be obtained. This, in turn, will accelerate battery research by providing the opportunity for a rapid evaluation of a wide range of design ideas and exploring different operating scenarios.

A creation of digital research and development platform requires accurate models that mimic physical batteries. For many years,

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**Abbreviations**

| | |
|---|---|
| ANN | artificial neural network |
| DNN | deep neural networks |
| DT | digital twin |
| ECM | equivalent circuit model |
| FNN | feed forward neural network |
| GPR | gaussian process regression |
| LCO | Lithium Cobalt Oxide |
| LFP | Lithium Iron Phosphate |
| LIB | Lithium-ion Battery |
| LSTM | long short-term memory |
| NMC | Nickel Manganese Cobalt Oxide |
| P2D | pseudo two-dimensional |
| RC | resistor-capacitor |
| SOC | state of charge |
| SOH | state of health |
| SPM | single particle model |
| SPTM | single particle thermal model |
| SVM | support vector machine |
| NDC | nonlinear double capacitor |

*Nomenclature*

| | |
|---|---|
| $i_0$ | Exchange current density |
| $t_+$ | Transference number |
| $D$ | Diffusion coefficient |
| $F$ | Faraday's constant |
| $I$ | Current |
| $R$ | Resistance |
| $R_g$ | Universal gas constant |
| $T$ | Temperature |
| $V$ | Voltage |
| $a$ | Specific surface area of electrode |
| $c$ | Concentration |
| $i$ | Current density |
| $r$ | Particle radius |
| $t$ | Time |
| $x$ | Spatial coordinate |

*Greek*

| | |
|---|---|
| $\kappa_D$ | Ionic diffusional conductivity |
| $\alpha$ | Charge transfer coefficient |
| $\varepsilon$ | Volume fraction |
| $\eta$ | Overpotential |
| $\kappa$ | Ionic conductivity |
| $\sigma$ | Electronic conductivity |
| $\varphi$ | Potential |

*Faraday's constant Subscripts and superscripts*

| | |
|---|---|
| $L$ | Load |
| $OCV$ | Open circuit voltage |
| $a$ | Anode |
| $app$ | Applied |
| $avg$ | Average |
| $c$ | Cathode |
| $cp$ | Concentration polarization |
| $e$ | Electrolyte phase |
| $eff$ | Effective |
| $ep$ | Electrolyte polarization |
| $eq$ | Equilibrium state |
| $k$ | Cell parts, $(k = n, sep, p)$ |
| $n$ | Negative electrode |
| $p$ | Positive electrode |
| $s$ | Solid phase |
| $surf$ | Surface |

electrochemical-thermal models, as one of the most accurate simulation methods available, have been used to study battery behavior using mathematical equations [13]. These electrochemical-thermal models are ideal for testing battery design ideas in a digital environment and can be developed further into battery digital twins [14].

In this context, a digital twin (DT) is defined as a virtual dynamic model that replicates the behavior of a physical entity [15]. Based on sensor data or historical data, DTs are commonly used to determine a system's control strategy [16–21]. However, DTs can also be used in the design and development of different systems [22]. This is because DTs can analyze system's behavior and determine the effect of different parameters on the performance of the system [23,24]. Many advantages can be derived from this technology, including improved performance estimation and behavioral prediction, reduced costs, and lower development risk [24].

It is imperative that the underlining models of a LIB DT are highly detailed in order to calculate local battery parameters with a high degree of accuracy [25,26]. To improve the quality of any model findings, it is necessary to incorporate large experimental datasets for parameter extraction and validation. Coupled partial differential equations describing mass and charge conservation and electrochemical reaction kinetics involving multiple electrical and electrochemical parameters such as electrical conductivity and diffusion coefficients must then be solved simultaneously in electrochemical-based models of the DT [27,28], which requires a significant amount of computation, particularly when thousands of iterations are required to obtain the optimal design.

Data-driven models and in particular machine learning algorithms offer better computational efficiency compared to physics-based battery models. By analyzing large experimental datasets or synthetic data from simulation results, these algorithms may be able to learn the physics of the LIB and may also act as a surrogate for the electrochemical-based DT. By combining the physical insight provided by the electrochemical-based DTs with the ML's fast response, the complementary advantages of each approach can be leveraged. This will allow us to develop an efficient DT that can be used to conduct battery experiments, digitally. The ML can be used for different applications, such as real-time parameter estimation, correcting errors of simplified battery models and for finding design related parameters to achieve optimal battery performance for a particular application when combined with optimization algorithms.

Physics-based machine learning can be applied to identify the complex relationship between important battery parameters across a range of battery length scales (from material to pack) and lifecycle stages (from production to end-of-life operation) for reducing the cost of production, enhancing battery performance and improved decision making for battery control [29–32] (Fig. 1).

In this work, the current state-of-the-art in battery modelling and machine learning to enable the development of a LIB DT is outlined. The work then explores the possibilities for developing a fully functional battery DT that can be used to optimize battery design. This work presents a review of studies towards application of machine learning for advancing the digitalization of battery experimentation. The novelty of this work allows the consolidation of studies in battery digitalization to focus the field on future research into digital experimentation. Moreover, this work consolidates this field to guide focus towards a goal of real-time battery monitoring and control, and digital battery research and development. The work gives clear gaps and perspectives of the field where focus on future studies and opportunities can lead to innovation

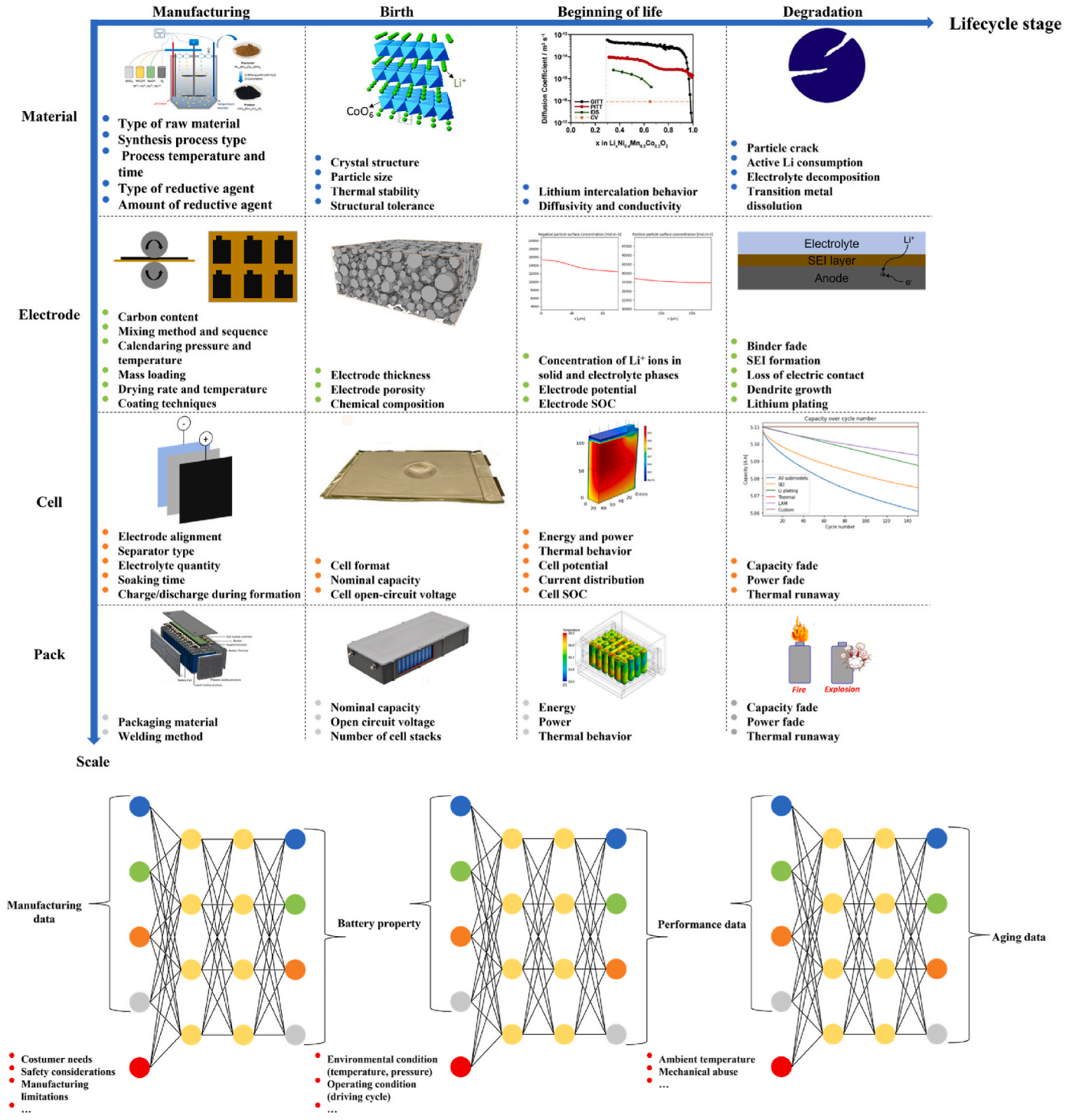


**Fig. 1.** Illustration of the interdependence of multiscale battery parameters across the entire battery lifecycle.

in digitalization of battery experimentation. The aim is that the opinions and perspectives presented in this work will lead to development of digital tools that can help monitoring and control of batteries, evaluation of innovative ideas, and accelerate the evolution of LIB industry.

### *1.1. Methodology*

With consideration of the types of modelling approaches for LIBs, the main physics-based modelling methods used include equivalent circuit models and electrochemical models. Additionally, machine learning approaches are utilized to predict unknown parameters, and to assess battery characteristics that may be computationally heavy for modelling approaches. These machine learning approaches include equivalent circuit models and electrochemical models. All these modelling and machine learning approaches are defined to assess batteries for specific applications and requirements. Considering the focus on performance of LIBs in this work, physics-based models and machine learning methods are discussed.

This work was performed to understand the pros and cons of the different modelling and machine learning approaches when considering battery monitoring and control, and battery design. Therefore, the suitability of these approaches has been evaluated. The following

methods were followed for the review of modelling and machine learning approaches.

- Collection of current applications of modelling and machine learning in LIBs towards monitoring, control, and battery design.
- Use of graphical-based analysis and comparison for modelling and machine learning applications in LIBs.
- Interpretation of the current state-of-the-art.
- Future predictions and trends in the field.

In general, a comprehensive review has been conducted with a thorough investigation of previous studies of modelling and machine learning in LIBs. A state-of-the-art review is provided for understanding modelling and machine learning used in LIBs. Based on the analysis, result interpretation is performed, and key findings are summarized. Finally, the future outlook and conclusions are presented.

This work is limited by the availability of published modelling and machine learning documentation. There are many private institutions where monitoring, control and design of batteries is a key aspect of their research and development portfolios. Developments in this field are therefore propriety information that is not shared in the public domain. Therefore, this work focuses only on available methods and studies that have been published.

Error can also be induced within this work. Modelling of LIBs relies on the use of many parameters that are defined experimentally, and some that are define theoretically. The misuse of parameters within a model of an LIB can cause errors in the results obtained. Furthermore, when incorporating the design of novel LIBs, the parameters determine both experimentally and theoretically may no longer be relevant. This would require experimental validation to ensure minimal errors.

## 2. Physics-based modeling of lithium-ion batteries

In LIBs, energy is converted between chemical and electrical energy through electrochemical reactions occurring within the active material of the electrodes [3]. To maintain electro-neutrality, electrons flow through an external circuit while $Li^+$ ions flow through the electrolyte from one electrode to another. Migration and diffusion are two processes that govern mass transfer due to gradients in potential and concentration, respectively [33]. During the operation of a LIB, charge transfer and electrochemical reactions produce heat. Also, some irreversible processes, such as formation of solid-electrolyte interface layer, lithium plating and particle fracture caused by diffusion induced mechanical stress occur [34]. Capacity loss, power loss and increased internal resistance are some of the observable effects of these undesired reactions [35].

These dynamic processes of the battery can be estimated in a model using mathematical equations and simplifying assumptions. Models of batteries can be very simple representations of the underlying system or they can be very detailed explanations of the mechanisms involved [36, 37]. A description of the most famous LIB models with different prediction capability and computational requirements is provided.

### 2.1. Equivalent circuit model

In equivalent circuit models (ECMs), circuit elements such as voltage sources, resistors and capacitors are combined to reflect the voltage variation of the LIB with regards to an applied current [38]. These models have simple structure with low computation time [39], are easy to implement and can have different form and components depending on the required application [40].

The simplest type of ECM is called Rint model consisted of an ideal voltage source in series with a resistor. The voltage source represents the OCV and the resistor is equivalent to the internal resistance of the cell which is caused by different battery and also side reactions [41].

Rint model only considers ohmic polarization which reflects the instant changes in voltage [42], therefore it is not suitable for practical applications [43]. For a more realistic simulation of voltage behavior, gradual changes due to other polarization effects also need to be considered. These polarization effects can be represented by parallel resistor-capacitor (RC) networks to the original Rint model.

Thevenin model comprises of a parallel RC network in series with other Rint model components. This additional RC pair accounts for electrochemical (activation) polarization which is associated with charge transfer [44]. The resistor represents the charge interfacial transfer resistance [45] while the capacitor is related to the double layer capacitance [46]. Thevenin model considers both ohmic and electrochemical polarization therefore it can better describe the transient behavior of the battery [47].

A second RC network is added to the Thevenin model in the dual polarization model to represent concentration polarization caused by gradients in the electrolyte and solid phases [48]. In this RC network, the resistor and capacitor account for concentration resistance and capacitance [49], respectively. Since this model can describe ohmic, electrochemical and concentration polarizations, it can generate accurate results [50]. The schematic of these model is shown in Fig. 2.

By addition of more RC networks the accuracy of the model would also be increased, but at the same time the computational efficiency would be lower [51]. ECMs could not be used for describing the spatial parameters of the battery such as ion transport behavior, but they are powerful tools for state of charge (SOC) estimation [52].

As the complexity of ECMs escalates with additional RC networks, and computational efficiency diminishes. Despite their performance in estimating SOC, ECMs exhibit limitations in characterising spatial parameters like ion transport behavior within the battery. The advantages of ECMs include providing a simplified yet practical approach to simulate LIB voltage variations. Therefore, there is a trade-off between model complexity and computational efficiency, emphasizing the suitability of ECMs for SOC estimation while highlighting their inability to capture intricate spatial battery dynamics. Although ECMs can be suitable for real-time monitoring of basic battery parameters, they are not able to be employed for digital battery research and development.

### 2.2. Electrochemical models

A LIB model based on electrochemical principles is more suitable for LIB research since it provides more detailed insight into the electrochemical behavior of the battery by describing the cell's galvanostatic charge and discharge processes, as well as transport phenomena. This kind of modeling also, allows tracking of the battery's spatial and temporal state, and provides estimation of parameters that are difficult to measure (e.g., $Li^+$ concentration) [53].

A common electrochemical model is the single particle model (SPM) proposed by Zhang et al. [54] as shown in Fig. 3. Taking each electrode as a spherical particle, this SPM model describes how Li ions diffuse within electrode spheres based on Fick's second law for spheres, as well as charge-discharge kinetics based on Butler-Volmer equation [55]. This means that Li diffusion within the spheres are considered as the governing process of the system while $Li^+$ concentration in the electrolyte is assumed to be constant [56]. This model is relatively fast, but does not provide detailed information regarding the processes occurring within the battery, and the battery's net response is only reliable at low current rates [57]. The electrolyte dynamics including electrolyte concentration and potential distribution have been taken into account in order to improve the accuracy of the conventional SPM model [58–60].

The Pseudo-two-dimension (P2D) model is a more comprehensive electrochemical model proposed by Doyle Fuller and Newman. In this model, electrodes are described as porous environments containing many spherical particles, with electrolyte filling the spaces between particles [61]. This model is schematically illustrated in Fig. 4. P2D model, describes concentration and potential variations in both electrode and electrolyte phases. Li ion diffusion in solid phase and

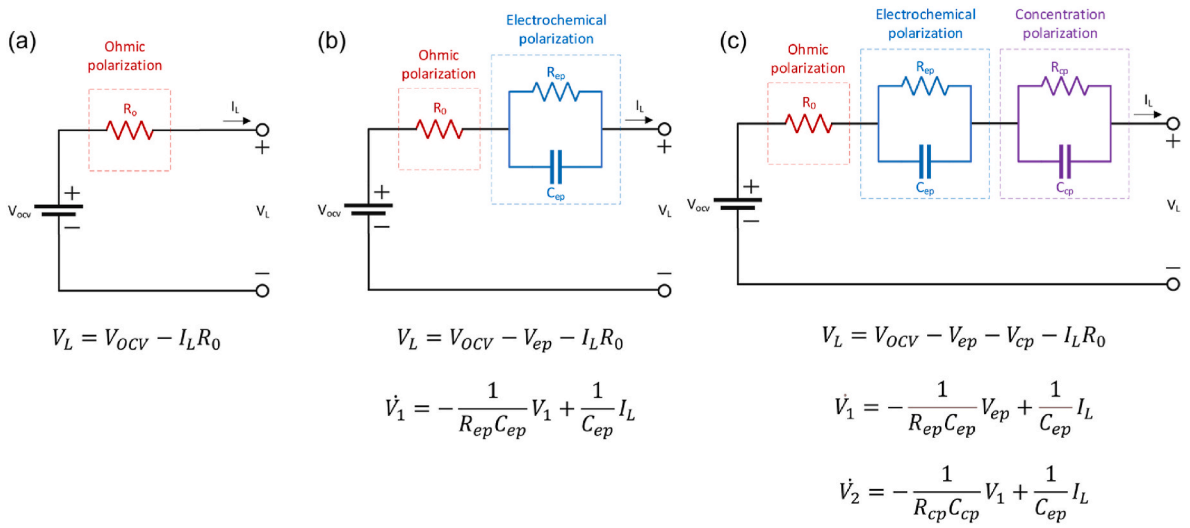


**Fig. 2.** schematic illustration of common ECMs. (a) Rint model, (b) Thevenin model, (c) dual polarization model.

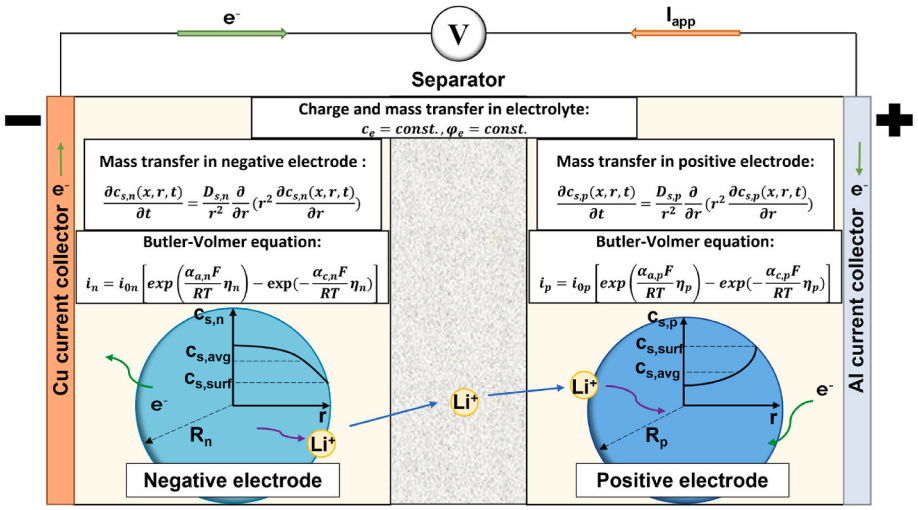


**Fig. 3.** Schematic illustration of SPM during discharge.

charge-discharge kinetics follow the same physical rules as the SPM. The equation for Li ion concentration has been derived from the general law of mass conservation [62]. The electrode and electrolyte potential equations are both governed by Ohm's law, although the electrolyte potential equation has an additional term which incorporates the effects of Li ion concentration [63,64]. The P2D model provides more detailed insight of the electrochemical behavior of the battery compared to SPM; but it also requires more computation time.

For a more realistic simulation result, it is possible to incorporate thermal and aging models into the original equations of the electrochemical models. Gu et al. [65], developed a multi-physics electrochemical-thermal model by integrating the P2D model with a thermal expression. In the proposed thermal model, heat generation was assumed to be caused by electrode reactions and Joule heating. This has been used for investigation of electrochemical-thermal behavior of LIBs [66–68], and simplified thermal models have been proposed to reduce the computation cost [69].

Degradation elements by Ramadass et al. [70] have also been integrated, allowing investigation of SEI formation on capacity fade [70]. Comprehensive electrochemical-aging models have also been developed [71,72], as well as electrochemical-thermal-aging models capable of considering the effect of temperature rise and degradation on electrochemical behavior of LIBs [73–75]. Data-driven models based on onboard measurable data [76], and empirical equations for estimation of battery parameters are also used for capturing modes of degradation in batteries [77,78], and have been integrated with electrochemical models [79]. Further additions to the P2D model include Li ion intercalation-induced stress for a $Li_yMn_2O_4$ positive electrode [80], electrochemical-thermal-mechanical stress [81,82], and a electrochemical-thermal-aging-mechanical model considering the effect of SEI formation, lithium plating and mechanical stress on solid particles [83].

A three-dimensional model of battery behavior facilitates enhanced insight, especially regarding heat generation and temperature distribution [84]. A 3D electrochemical-thermal model was developed for a standard 18650 cell [85]; whereas, Fang [86] used a 3D electrochemical-thermal model to simulate the Nail-penetration test [87] for internal short-circuit investigation. Such models have been used for thermal analysis of different LIB formats, including pouch and prismatic cells [88,89]. Additionally, three-dimensional modeling was used to simulate the electrochemical behavior of an LIB cell with a heterogeneous negative electrode consisting of solid particles of different shapes and sizes [90].

Considering the models developed to describe LIBs' processes with

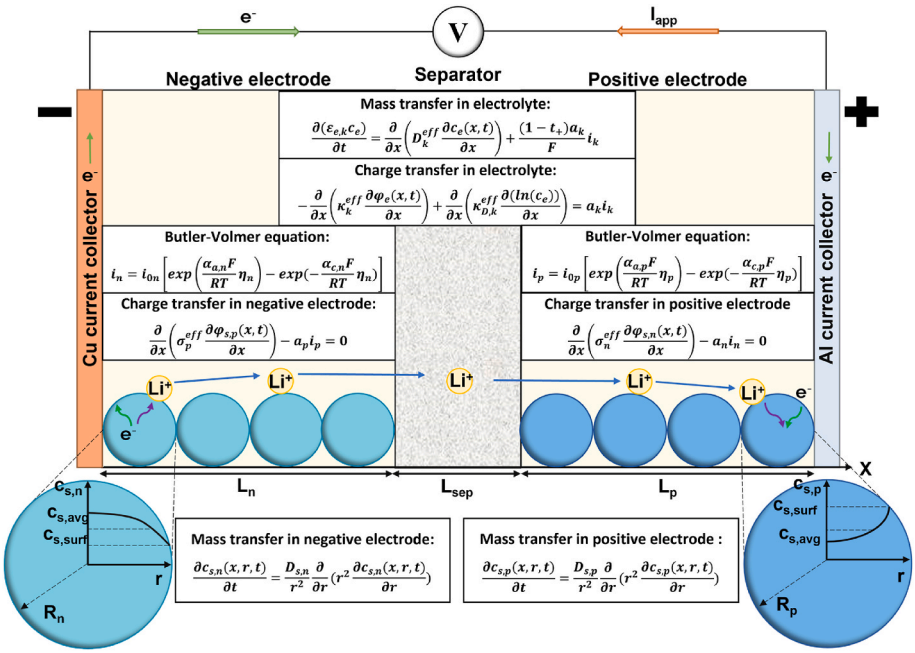


**Fig. 4.** Schematic illustration of P2D model during discharge.

high level of accuracy. It is becoming possible to move the digital models closer to the physical entities due to their maturity and reliability. By transferring all aspects of LIBs to a digital environment and developing a model with in-depth details, it is possible to develop a LIB DT. This involves transferring all aspects of LIBs, including electrochemical, electrical, thermal, aging, and mechanical, to a digital environment [91]. Developing such a multi-physics DT requires careful parameterization and validation based on extensive test data of LIBs. Such DT can also be developed with the aid of powerful computational resources and battery simulation packages, such as PyBaMM [92], COMSOL [93,94], and LIONSIMBA [95]. However, such a DT will be computationally expensive due to the high number of complicated equations that need to be solved simultaneously. Despite this, any simplification that reduces the cost of computation, such as ignoring side reactions will lead to deviation from the reality. Therefore, it is important to come up with methods of reducing the computational cost without sacrificing accuracy and detail.

The prospect of developing a DT for LIBs, amalgamating electrochemical, electrical, thermal, aging, and mechanical aspects into a unified digital environment, holds promise. However, achieving this requires precise parameterization and validation against extensive experimental data, which can be challenging to verify and cross-correlate between multiple studies due to the different methods used to obtain experimental data.

The significance of electrochemical models in elucidating LIB behavior is clear, due to their capacity to capture detailed electrochemical phenomena and their crucial role in understanding LIB performance. However, there are many challenges associated with computational demands, model complexity, and the quest for balancing computational efficiency without compromising accuracy. Despite this, these models represent a pathway toward accurate digital representations of LIBs, albeit with complexities in computational execution and the need for continued advancements to enhance accuracy and efficiency. This allows the use of electrochemical models for digital design and research, but requires substantial computation power and time, preventing them from being utilized in real-time applications and impeding the development of LIB DTs.

## 3. Machine learning approaches for lithium-ion battery applications

The use of machine learning in the technology sector has been widespread for quite some time [29,96]; however, ML in batteries has only gained traction in the last decade. For effective ML parameterization and performance prediction for different battery materials, structures, sizes, and formats, the emergence of advances in sensing technologies and experimental tools [97,98] has benefited the field of battery modelling by improved parameterization and reduced computational requirements [20]. Moreover, the application of ML in the battery field has gained significant importance due to the effectiveness of ML methods in reducing the requirement for experimental approaches [99].

Different types of artificial neural networks (ANN) including feed forward neural networks (FNN), deep neural networks (DNN) and recurrent neural networks (RNN) such as long short-term memory (LSTM), support vector machine (SVM), gaussian process regression (GPR), decision tree and random forests [96,100,101] are commonly used ML approaches for LIB estimation and performance prediction [102–104]. Fig. 5 shows the structure of some of these algorithms.

Table 1 provides information on the findings of studies that investigated ML models for LIB applications. FNN has proven to be a suitable choice for studying the relationship between material and cell properties and the resulting battery performance. Meanwhile, RNN, LSTM and GPR methods have been extensively used for online estimation of time-dependent battery states such as state of health (SOH) and SOC estimations. GPR is a suitable choice for capacity estimation which can be trained with small dataset, but the complexity of the model has shown to be a challenge. SVM stands out as a simple and accurate model when it is used for regression tasks, providing efficiency comparable to NNs. Both DT and RF have been successfully employed for both classification and regression tasks.

It is, however, very difficult to provide a general comparison on the performance of each ML model across different LIB applications since the predictions of these models are dependent on the training dataset. It is only possible to provide such comparison when different models are trained with the same dataset and for the same task. Many comparative studies have done such investigations across different ML algorithms. Li

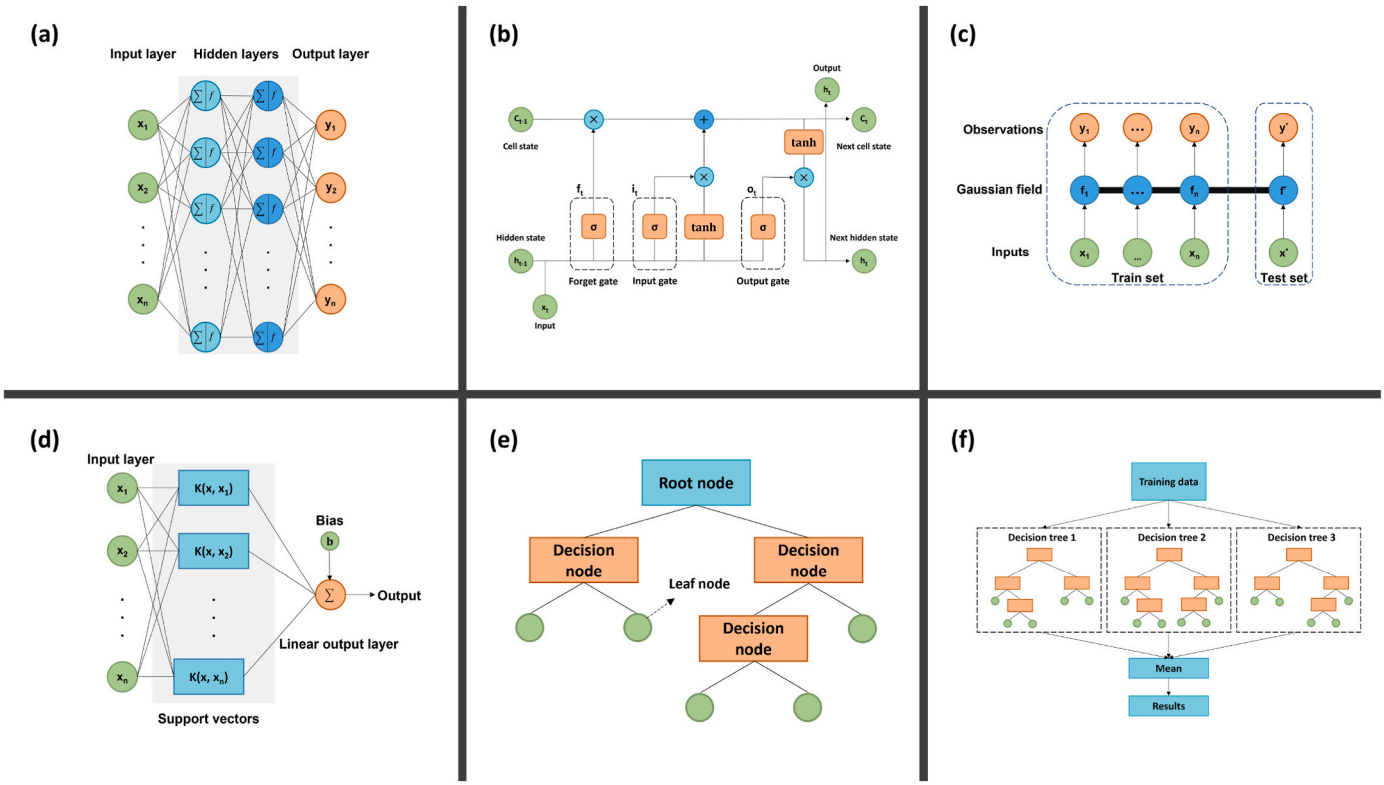


**Fig. 5.** Structure of commonly used ML algorithms in LIB applications. (a) Neural networks, (b) LSTM, (c) GPR, (d) SVM, (e) random forests, (f) decision tree.

et al. [118] compared prediction accuracy and computational efficiency of GPR and RF for capacity estimation. The results showed that RF and GPR are both capable of accurately predicting the capacity with a root mean squared error (RMSE) of 0.82 % and 1.16 %, respectively. In addition, RF showed to be at least ten times faster than GPR, indicating the superior capability of RF for online SOH estimation. Zhang et al. [111] developed a LSTM model for RUL prediction of LIBs. The goal was to predict the number of cycles that a battery could undergo before the capacity falls below 80 % of the initial capacity using the data from previous cycles. The prediction capacity and computational time of the LSTM was compared to SVM and a simple RNN model for four different cells. The three models showed better results when larger training data was used. In all cases, the computational time of the SVM model was the lowest (less than 0.01s), while the RNN took the longest to be trained (about 40s). SVM showed superior predictive capabilities compared to simple RNN by predicting the failure cycle closer to the actual values. In contrast, RNN failed in capturing the long-term dependencies of capacity degradation. Overall, LSTM showed better prediction capacity compared to both SVM and RNN with a reasonable training time of around 20s. Sahinoglu et al. [113] developed four GPR variants for battery SOC estimation utilizing voltage, current, and temperature data, along with SOC values from prior cycles. They performed a comparative analysis by evaluating the performance of the GPR models, a NN and a SVM model. All GPR variants showed lower RMSE compared to NN and SVM with NN outperforming SVM. The computational time for GPR models was higher than the other two but still sufficiently low for real-time SOC estimation applications. Liu et al. [119] performed a multi-class classification using a RF model to find the correlation between manufacturing features from coating and mixing stages with battery porosity and mass loading. The accuracy of the developed RF model was compared to a DT and a SVM model. The DT showed the weakest accuracy, while SVM results were very close to RF predictions.

Standardizing the dataset used for ML application in LIBs facilitates meaningful comparisons across various studies. This involves defining specific guidelines for test procedure, measurement methods, and the required input data. In addition, a standard framework of reporting the information such as properties of the tested batteries and utilized equipment and an agreed-upon grading system for dataset quality allows researchers to use consistent train and test datasets. This approach minimizes the diversity in the datasets, making it easier to compare the performance of ML approaches; therefore, any differences in performance could be attributed to the models themselves.

ML algorithms are dependent on experiential data, which is labor-intensive, expensive, and time-consuming to acquire. Additionally, these algorithms cannot provide physical insight into the system when trained based on the measurable data obtained from battery experiments (voltage, current, temperature) since the system is regarded as a black box, meaning it treats data solely based on statistical analysis. To be able to utilize the information obtained from these methods to enhance LIBs performance, it is necessary to understand the underlying physical mechanisms. Combining physics-based and data-driven models could be the solution to this problem.

The main idea here is to inform the ML algorithm of the physical relations inside the system so that it can map the inputs directly to the corresponding outputs without having to solve complex non-linear equations in each iteration. This way, accuracy will always be above 90 % while results are achieved much faster [120]. As a result, it will not be necessary to simplify the electrochemical model's governing equations. Moreover, large experimental datasets will be eliminated when they are only required during model development, eliminating the need for such datasets. By incorporating ML algorithms, it is possible to develop an extensive, computationally inexpensive LIB DT that can be applied to battery modeling and control, as well as battery design and development. As an overview of the state-of-the-art in physics-based machine learning for LIBs, the following examples are presented.

## 4. State-of-the-art in hybrid methods for batteries

Hybrid modeling is referred to a novel modeling approach in which the machine learning algorithms are integrated with physics-based

**Table 1**
A summary of machine learning approaches for lithium-ion batteries applications.

| Machine learning approach | Application | Challenges | Outcomes | Reference |
|---|---|---|---|---|
| FNN | Electrode material design | •Small available dataset<br>•Large number of input features<br>•Significant error for some data points at low redox potential | •Redox potential prediction with average error of 3.54 %<br>•Ranking the importance input features | [105] |
| | Electrode mass balancing | •Limited available experimental dataset | •The model could predict capacity of the battery for different current densities and active material mass ratios with average error of 2 $mAhg^{-1}$ | [106] |
| RNN | SOH estimation | •Utilized a large dataset from months of experiments | •Capacity and resistance prediction with an MSE of 0.462 and 0.296 | [107] |
| | SOC estimation | •Required careful hyperparameter selection.<br>•Higher error at longer discharge times | •SOC estimation under different working condition with a prediction error of 6 % | [108] |
| LSTM | SOC estimation | •Complexity of problem due to strong relation between SOC and SOH | •SOC estimation with maximum error of 0.016 | [109] |
| | SOH | •Difficulty in hyperparameter selection<br>•Need for eliminating the redundant information | •SOH estimation with 2 % RMSE | [110] |
| | RUL | •Need for regularization method to prevent overfitting | •Better prediction capability compared to SVM and simple RNN.<br>•RUL prediction based on a small portion of online data (20–25 %) | [111] |
| GPR | Capacity estimation | •Contrasting results of model performance with regards to selected features when different datasets were used for training | •2–3% prediction RMSE by using small voltage curve segments (10s) | [112] |
| | SOC estimation | •Both current and previous system states had to be used for accurate prediction | •Higher computational time and lower prediction error compared to SVM and NN | [113] |
| SVM | Prediction of crystal system | •Difficulty in classifying the data due to lack of cathode structure | •Correlation between the crystal system and cathode properties were found.<br>•Lower prediction capability compared to NN and RF | [114] |
| | SOH estimation | •Several feature selection methods were used but a significant improvement was not achieved | •Slightly lower accuracy compared to NN but lower complexity | [115] |
| DT | Lifetime estimation | •Small available dataset<br>•Large number of features | •Highest accuracy (95.2 %) compared to other algorithms such as GP and SVM to predict if the battery can maintain 80 % of capacity after 550 cycles | [116] |
| | Cycle life prediction | •Large number of features | •7 % error in lifetime prediction<br>•Better prediction capacity compared to SVM, GPR, RF and simple DT | [117] |
| RF | Capacity estimation | •Cycling test of several cells under varying condition<br>Selecting the most suitable features | •Capacity estimation of different batteries with RMSE of less than 1.3 % | [118] |
| | Manufacturing | •Difficulty of collecting manufacturing data across all stages | •F1 score of 90.1 % for mass load.<br>•F1 score of 66.4 % for porosity.<br>•Ranking the importance of each feature | [119] |

models to harness the advantages of both methods. By combining the ability to learn the complicated patterns and fast computational capabilities of machine learning models with high predictability of physics-based models, a more flexible and robust framework for LIB research can be developed.

A variety of hybrid methods for modelling batteries must be developed and utilized to achieve a truly intelligent LIB DT. The purpose of this section is to describe selected hybrid methods for monitoring and controlling batteries. An overview of studies using hybrid methods to assess LIB design follows. Combined, these studies give us the foundation for building an intelligent LIB DT that can be used as a digital LIB lab.

### 4.1. Battery monitoring and control

#### 4.1.1. Performance prediction

P2D model can accurately predict battery dynamic behavior of the battery during operation but it is computationally expensive for real-time application. There have been efforts to reduce the time of this model to enable the implementation of it for battery management purposes.

Dawson-Elli et al. [121] proposed a combination of a comprehensive pseudeo-two-dimensional model with a variety of ML algorithms including decision trees, random forests and gradient boosted machines to evaluate their execution time and accuracy. Using the P2D model, a dataset containing 24000 parameter combinations with variations across 27 parameters was created. All approaches had reasonable accuracy in predicting the voltage of the next time step using the four previous time steps during constant current discharge; however, the models were unable to predict voltage values for different current rates or battery chemistries rather than that of the training dataset. SOC prediction yielded low accuracy due to the high variances in the dataset, suggesting that the dataset should be restructured and comprehensive ML algorithms should enhance the results [121].

In another work by Li et al. [122] a modified version of LSTM called two-dimensional grid LSTM was used to map measurable battery data to internal spatial-temporal states. To generate training and test datasets, an electrochemical-thermal model was utilized. Using a SOC ranging from 5 to 95 %, and operating temperatures ranging from 0 to 40 °C, fifteen EV drive cycles were used as inputs for the P2D model. By utilizing different voltage, current and ambient temperature values, the physics-informed LSTM was able to predict internal LIB internal states. These states included average and surface $Li^+$ concentration and potential in the electrode and electrolyte, which are essential for battery state estimation, safety, and lithium plating. A maximum error of 3.95 % was observed in the prediction of internal states using the proposed model when noisy input data was used.

A schematic illustrating the proposed flowchart of these works is represented in Fig. 6.

It is also possible to increase the accuracy of simple physics-based models such as SPM and ECM by combining them with machine learning algorithms using a hybrid architecture as shown in Fig. 7.

Tu et al. [123] proposed hybrid models by integrating physics-based models and a FNN algorithm. The goal was to enhance the prediction accuracy of a single particle thermal model (SPTM) and an ECM. The FNN was employed to capture voltage deviations between these models and the true voltage value. In the SPTM-FNN hybrid framework, the neural network is trained based on a simulated dataset generated using a full-order P2D model of an LCO-graphite cell. The current profile, initial SOC, and initial temperature were fed to the SPTM, to calculate bulk and surface SOC, and temperature profile as the outputs. The hybrid SPTM-FNN framework produced impressive improvements in prediction accuracy compared to the SPTM. Using experiments conducted on Samsung INR18650-25R LIB cells, the required variables for an ECM model called nonlinear double capacitor (NDC) as well as the training dataset for the FNN algorithm were derived. The initial SOC and current profile are inputs to the NDC model. The outputs include the voltages of the bulk inner regions of the electrode, electrode surface voltages, and transient voltages resulting from ion diffusion. These outputs and the current and temperature profiles were fed to the FNN to calculate the modified voltage. The NDC-based hybrid model has been enhanced to capture the effect of aging on battery voltage response. The proposed framework produces significantly lower voltage errors than the NDC model at all current rates by including state of health as an additional input to the FNN.

For the accurate prediction of battery voltage and temperature, Feng et al. [124] have developed an electro-thermal neural network (ETNN). Based on surface temperature and current, an electrochemical-thermal sub model (ETSM) was applied to estimate terminal voltage and core temperature. The neural network was trained based on experimental dataset to capture the voltage residuals therefore the ETNN was able to deliver high precision under high C-rates (up to 10 °C) and wide temperature ranges (−10 to 40 °C). The inputs to the neural network were the measured current and estimated voltage, and core temperatures from ETSM. Using an unscented kalman filter, a maximum RMSE of 0.9 % was obtained at 40 °C for estimating SOC and 1.08 °C for estimating state of temperature at −10 °C.

Combining electrochemical models with ML techniques to enhance accuracy and reduce computational load in predicting LIB performance is a promising route towards LIB DTs. However, there is an ongoing requirement to optimize these hybrid models for accurate and efficient LIB modelling. Despite this, there is substantial potential of combining physics-based models with ML algorithms for improved LIB performance management.

#### 4.1.2. Parameter estimation

Combining P2D with thermal and aging models can provide an understanding of how battery parameters change during operation. While such a comprehensive model may take a considerable amount of time to run the use of machine learning can assist this model to make real-time predictions.

An LSTM algorithm was also developed by Chun et al. [125] for real-time parameter estimation. The algorithm was trained to replicate the dynamics of a Nickel Manganese Cobalt Oxide (NMC) LIB cell using synthesized data of measurable parameters including, voltage, current, temperature, and SOC generated with a P2D model combined with thermal and aging models. This study considers anode electrolyte decomposition, cathode electrode decomposition, and battery volume change phenomena, which affect solid particle surface area and solid

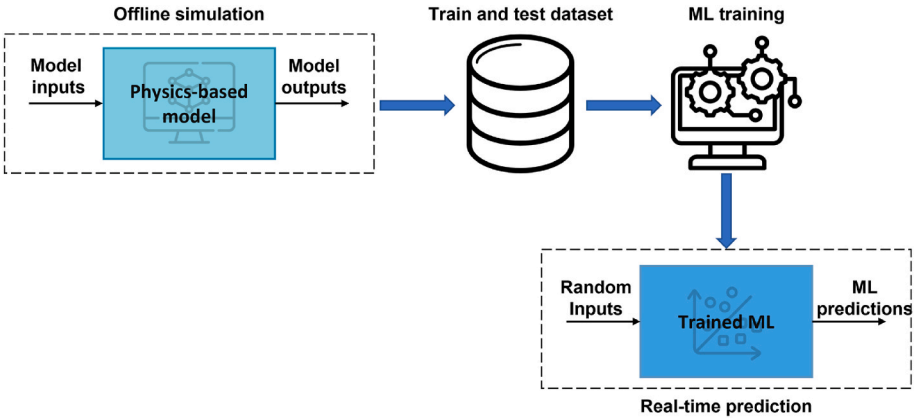


**Fig. 6.** Workflow of hybrid models for dynamics training.

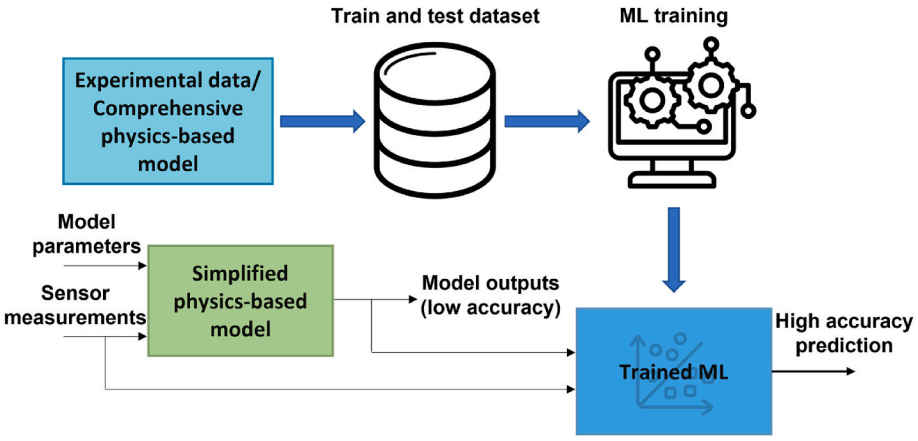


**Fig. 7.** Workflow of hybrid models for improved prediction accuracy.

particle conductivities for anode and cathode, normalized available capacity, and SEI layer thickness battery parameters. The training dataset was created by applying variations in the aging-related parameters. The trained LSTM network was validated using experimental data from an NMC battery cell test. The experimental data included voltage, current, and temperature, while SOC was computed using the Coulomb counting method. This data was used as the input of the LSTM network to estimate aging-relevant parameters, where simulated voltage results matched experimentally obtained voltage results with an RMSE of 0.43 %. The proposed parameter estimation workflow of this work is represented in Fig. 8.

In Table 1, this work summarize the existing research on physics-informed ML for battery control and monitoring, the models involved, the ML methods applied, the method of generating training data, the battery chemistry, and the application of the developed hybrid model.

There is an increasing interest in utilizing ML techniques for parameter estimation and real-time predictions in LIB systems. The effectiveness of ML algorithms, such as LSTMs, in estimating crucial LIB parameters, enhancing the accuracy of predictions, and enabling real-time monitoring and control is promising. This underscores the potential of combining physics-based LIB models with ML algorithms for accurate parameter estimation and efficient LIB management.

### 4.2. Battery design

Hybrid models can be extremely beneficial when it comes to battery design, where complicated models must be run several times before the desired result is achieved. In Fig. 9, a general workflow is shown for combining physics-based models with machine learning algorithms for LIB design applications. Various applications of hybrid models are discussed in this study.

#### 4.2.1. Improved energy and power

A thermal-electrochemical model was combined with neural network algorithms in Wu et al.'s [126] study to determine the optimal design of an NMC-graphite cell to achieve high specific power and specific energy. Electrode thickness, volume fraction, Bruggeman constant, active material radius, and lithium concentration in the electrolyte were selected from those parameters of the positive electrode that can be controlled during manufacturing. For the proposed method, two neural networks were used. The first one served as a classifier that assessed whether an input parameter set was physically feasible. In this neural network, the six design parameters were inputs. As the algorithm's output, a value ranging from 0 to 1 was generated, with 0 representing an abnormal input. A second neural network was used to calculate the specific power and specific energy of a given set of inputs. While C-rate is the most important factor affecting specific power, electrode thickness and porosity are the two most important factors affecting specific energy. To obtain optimal design parameters that satisfy both the requirements for high specific power and energy, a total of 10000 Monte Carlo algorithms were performed on the trained networks.

For a LIB with thick electrodes, Gao et al. [127] obtained an optimized electrolyte channel design, improving battery performance during fast charging and mechanical stability. Their study used electrochemical and mechanical models, deep neural networks, and Markov Chain Monte Carlo. To determine the effect of geometric

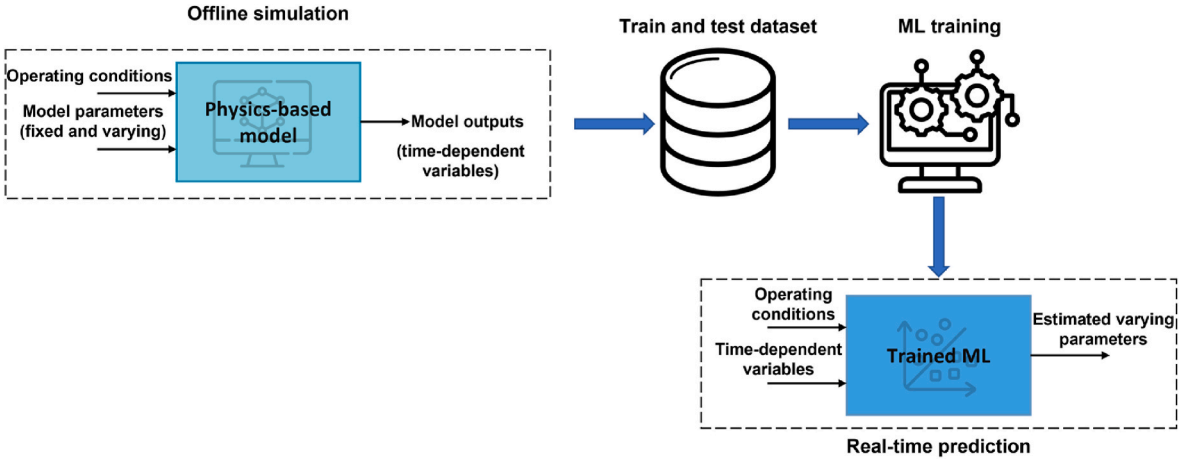


**Fig. 8.** Workflow of hybrid models for parameter estimation.

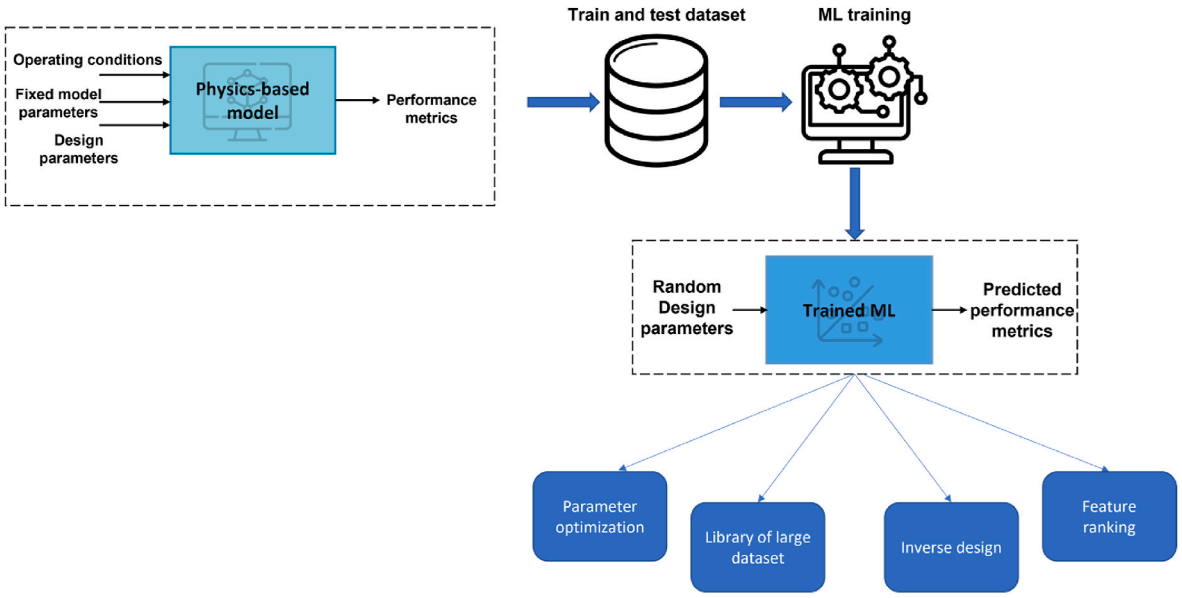


**Fig. 9.** workflow of integration of physics-based modeling and machine learning for LIB design applications.

parameters on cell performance, simulations were conducted using the electrochemical and mechanical model. Various electrolyte channel lengths and widths, and electrode material widths were simulated. Each set of simulations compared specific energy, power, capacity, and mechanical stability with conventional electrodes without channels. Data generated by simulation was used to train DNN. To obtain the optimal channel design, the trained DNN was combined with a Markov Chain Monte Carlo optimization algorithm. By varying the length, width, and tapering degree of the cathode and anode electrolyte channels, specific energy, power, and capacity contours were calculated. A maximum error of 1.94 % was calculated from Ragone plots of possible specific energy and power values. Furthermore, by freely modifying all six channel geometrical parameters and choosing specific energy as the design goal, the optimal channel design improved by 74 %.

A method developed by Deng et al. [128] for obtaining cathode active material distribution resulted in higher specific energy compared to an electrode with a uniform surface. To test the proposed method, they utilized an NMC-Li cell. In the NMC electrode, the average solid volume fraction was 50 %, and the rest was filled with electrolyte. Using a pseudo-three-dimensional model, cell energy was calculated by considering variations perpendicular to electrode thickness. DNN was used to learn the physics of the system and generalized simulated annealing was integrated with the DNN to find the optimal pattern. They fed the DNN with 100 values of volume fraction and their corresponding specific energy values based on the pseudo-three-dimensional model. The energy is calculated with the trained DNN instead of solving the equations of the electrochemical method, and a base value for volume fraction is calculated using generalized simulated annealing. A new set of volume fractions was then generated by adding noise to the base value. An updated training dataset was created with volume fraction values closer to the optimal region; therefore, training the DNN with this dataset would be more accurate. The optimal solid material distribution showed a periodic pattern with some channels filled with electrolyte, easing the transportation of lithium ions.

To improve ionic transport and reduce voltage drop during high charging rates, Sui et al. [129] proposed a bio-inspired vascularized electrode design. The proposed structure reduces the transport resistance near the separator, reducing voltage drop. Comparing the capacities of homogenous, vertical channel electrodes, two-branched and four-branched vascularized electrodes confirmed this hypothesis, with the vascularized electrodes showing the highest capacity. An artificial neural network was employed to find the optimal geometry. Based on 11 geometric parameters of the vasculature channels, a training dataset was generated. Each parameter combination represented a unique vascularized structure. COMSOL Multiphysics was employed to solve an electrochemical model with the finite element method (FEM). The final ANN model was 84 times more computationally efficient than the conventional FEM. By using the trained ANN's efficient prediction capability, a library of useful information was created to store charging curves, channel structure, charging rates, capacity, and porosity, as well as some electrochemical data, such as energy density, average voltage, and power density. Using this library, the optimal electrode structure design can be determined by defining manufacturing and operation limitations (channel radius, C-rate, and power density) and performance objectives. After successfully applying the vascularized graphite anode, the proposed structure was also applied to the cathode. The full cell vascularized structure showed a 66 % charging capacity enhancement compared to traditional homogenous electrodes.

The effectiveness of ML techniques in optimizing LIB designs for improved energy and power is a new and exciting frontier in LIB research. There is a clear synergy between physics-based models, ML algorithms, and optimization strategies in enhancing battery performance, providing novel insights into designing electrodes, electrolyte channels, and active material distributions. Such integrations enable the efficient exploration of vast design spaces, resulting in significant enhancements in LIB performance metrics, as demonstrated by these studies. However, as this field develops and expands, it is reasonable to assume that the digital LIB experimental space will transcend physical laboratory experimentation, leading to challenges in verifying results obtained digitally. Therefore, it is imperative that validation with physical experimentation is maintained to validate promising digital developments.

#### 4.2.2. *Improved thermal management*

A nail penetration model, ML regressor algorithm, and genetic algorithm were used in Yamanaka et al.'s [130] study to identify battery design parameters for higher safety. Through nail penetration simulations within the range of input variables, including cell design parameters, test conditions, and performance indicators, the training database was created. By multiplying the finite element parameters by 0.5 and 1.5, upper and lower limits were set for the design and test parameters. This method generated 368 datasets. Descriptors include electrical,

electrochemical, and dimensional parameters, and battery test conditions such as nail velocity, position, and diameter, while predictors include combustion volume, capacity, and averaged internal resistance. By analyzing the relationship between descriptors and predictors, correlation factors were calculated that indicate parameter dependency. For each predictor, a GPR algorithm was constructed. Using regression models, the values were predicted with high accuracy with a $R^2$ of 0.9 or greater. To find the design parameters leading to better performance, a genetic algorithm was used. Cell width, cell height, cell thickness, negative electrode layer thickness, negative active material diameter, negative porosity, and negative active material $Li^+$ diffusion coefficient were optimized, which resulted in 3.3 times greater capacity and 0.78 times lower internal resistance as well as a minimized combustion volume.

Li et al. [131] used a multilayer perceptron neural network to find the optimal battery pack configuration for enhancing battery thermal management. A 3D electrochemical model was used to simulate battery pack temperature distribution and heat transfer to the ambient environment. Nine pack configurations with variations in the gaps among battery pairs were formed. Each configuration's temperature distribution was analyzed under various operating conditions to create 130 datasets of inputs and outputs for the ANN. The inputs to the ANN included gap dimensions in two directions as the configuration parameters and air velocity and ambient temperatures as the operating conditions. The model outputs are the maximum temperature of a battery cell and the difference between its highest and lowest temperature. The developed hybrid model calculated 6,250,000 data of different battery configurations under various operating conditions and identified the optimal configuration. A 1.9 % reduction in maximum temperature and a 4.5 % reduction in maximum temperature difference improved battery cooling efficiency and performance.

The efficacy of ML approaches linked with LIB modelling methods has been shown to improve thermal management within LIB designs. This allows the improvement of LIB designs to optimize safety, temperature distribution, and cooling efficiency within LIBs. Although the application of ML-driven approaches demonstrates their potential in enhancing thermal management strategies, offering insights into optimal battery designs for improved safety and performance, further research should focus on improving the accuracy of these methods. In addition, there is still a requirement for these approaches to be applied to the knowledge gained from LIBs used in real-world applications considering the various climates and environments LIBs are routinely used in.

#### 4.2.3. Mesoscale design

In their study, Takagishi et al. [132] developed a physicochemical based data-driven approach to find the mesoscale structure of LIB electrodes, resulting in lower specific resistance and higher capacity and power. A simplified physicochemical model was used to simulate the specific resistance during charge-discharge processes for 2100 randomly generated 3D structures. Analyzing the model's results, the relationship between active material volume ratio, particle radius, matrix binder conductivity, additives volume ratio, and pressure in the compaction process was constructed. To create regressions between process parameters and total specific resistance, an ANN algorithm was developed. A Bayesian optimization method was used to find the optimal electrode structure. Electrodes with a 50 % volume ratio and a binder/additive volume ratio less than 0.1 % give lower total specific resistance than other electrode structures.

Kabra et al. [133] used physics-constrained ML algorithms to characterize electrode microstructural properties. A dataset of 17,000 electrode microstructures was generated by varying ellipsoidal particle shapes, sizes, orientations, and active material and binder phase composition. A 3D physics-based pore-scale simulation method was used to characterize these electrode structures. Electrode properties included effective electronic conductivity, tortuosity of the pore network in three directions representing $Li^+$ transport in the pore network, and volume-specific surface area, which represents the interfacial area for electrochemical reactions. The method was also applied to a graphite cathode, but it can be applied to other porous electrode materials as well. Based on the created dataset, linear regression, lasso regression, elasticnet, ridge regression, decision tree, adaboost, and gradient boost algorithms were trained to map physical descriptors (inputs) to electrode properties (outputs). Predictions of different properties were more than 90 % accurate.

A summary of hybrid methods used in research for LIB design applications on a variety of scales and objectives is presented in Table 2.

Optimizing electrode structures at the mesoscale is a promising route for improved LIB performance, where ML-driven modelling approaches are effective (see Table 3). The integration of physics-based models and ML algorithms has provided insights into the relationships between electrode structure and performance metrics in LIBs. However, there is a limitation in the validation of some approaches. Designing intricate structural changes digitally can yield performance gains but can be difficult to verify experimentally if there structure is not straightforward to engineer using current technologies. Although the state-of-the-art demonstrates the potential for ML techniques to guide the design of mesoscale electrode structures, thereby enhancing specific resistance, capacity, and power in lithium-ion batteries, there is still the requirement for further physical verification of these findings.

### 4.3. Hybrid modelling roadmap

Designing batteries utilizing hybrid modelling methods involving physics-based models and machine learning is an emerging field and requires a comprehensive approach. The authors suggest the following concise roadmap based on current research and future prospects.

Data collection and preprocessing is required to gather diverse datasets encompassing battery characteristics, performance, and aging under various conditions. It is imperative to ensure data quality, standardisation, and compatibility for subsequent modelling stages, allowing the adaptation of modelling results between fields. Physics-based modelling must be developed or refined into simpler models based on electrochemical principles, incorporating material properties, kinetics, and thermodynamics. These must be simplified so they can be integrated with machine learning algorithms for improved accuracy and efficiency in real-time. Machine learning integration into hybrid models requires the identification of appropriate machine learning techniques (e.g., neural networks, ensemble methods) for coupling with physics-based models. The machine learning methods must then be trained using the combined datasets (use by both the physics-based models and machine learning), leveraging machine learning to enhance predictive capabilities and model robustness.

Hybrid model validation and optimization using experimental and usage data to assess their accuracy and reliability. This can be challenging for designs that are not yet developed physically, and therefore lacking experimental data. This can be alleviated by optimizing the hybrid models iteratively, fine-tuning parameters and architectures for better performance. Following this, the application and scaling of hybrid models can be performed. This will involve the implementation of the validated hybrid models in practical scenarios for battery design, optimization, and predictive maintenance. This will also open opportunities for the models to be applied to broader applications across different battery chemistries and configurations. This will result in robust hybrid models that may give insight into designs of batteries that have not yet been validated experimentally.

Future research directions should focus on investigating novel data-driven techniques and advancements in machine learning for further improving hybrid modelling accuracy and efficiency. This includes the exploration of the integration of AI-driven optimization algorithms for advanced battery design, control, and monitoring. To achieve this, it will be required that many scientific disciplines collaborate in a

**Table 2**
Summary of works on hybrid methods for battery controlling applications.

| Reference | Physics-based model | ML method | Train and test dataset | Chemistry | Functionality |
|---|---|---|---|---|---|
| Dawson-Elli et al. [121] | P2D-thermal | decision tree, random forests, gradient boosted machines | Synthetic data from P2D-thermal | NMC | Terminal voltage and SOC prediction |
| Tu et al. [123] | P2D-thermal, SPM-thermal, ECM | FNN | Synthetic data from P2D-thermal and SPM-thermal, experimental data | LCO | Improving the accuracy of SPM and ECM |
| Feng et al. [124] | SPTM | FNN | Synthetic data from SPM-thermal, experimental data | LFP | Improving the accuracy of SPTM |
| Li et al. [122] | P2D-thermal | LSTM | Synthetic data from P2D-thermal | NMC | Internal battery state estimation under real-world condition |
| Chun et al. [125] | P2D-thermal model and SEI dynamic model | LSTM | Synthetic data from P2D-thermal and SEI dynamic model | NMC | Real-time parameter estimation |

**Table 3**
Summary of works on hybrid methods for battery design applications.

| Reference | Physics-based model | ML method | Scale | Design variables | Chemistry | Objective |
|---|---|---|---|---|---|---|
| Wu et al. [126] | Electrochemical-thermal model | ANN | Battery cell | Positive electrode thickness, volume fraction, Bruggeman constant and particle radius, electrolyte $Li^+$ concentration, applied C-rate | NMC | Improved specific energy, specific power, and specific capacity |
| Gao and Lu [127] | P2D and mechanical stress model | DNN | Battery cell | 6 geometric channel parameters | – | Improved specific energy, specific power, and specific capacity |
| Deng and Lu [128] | pseudo-three-dimensional | DNN | Battery cell | Solid volume fraction | NMC-Li | Improved specific energy |
| Sui et al. [129] | P2D | ANN and the bagging ensemble algorithm | Battery cell | 11 geometric channel parameters | LCO | Improved capacity and charging time |
| Yamanaka et al. [130] | Nail penetration (coupled 1D electrochemical-2D electrical-3D thermal) | GPR | Cell stack | Cell width, height and thickness, negative material thickness, particle radius, porosity, and $Li^+$ diffusion coefficient | NMC | Minimized combustion volume and internal resistance, improved safety, and thermal management |
| Li et al. [131] | Simplified electrochemical model and lumped thermal model | Multilayer perceptron neural network | Battery pack | Gap between battery pairs | LFP | Enhance battery thermal management |
| Takagishi et al. [132] | 3D structure simulation, Simplified physico-chemical model | ANN and Bayesian optimization | Electrode mesostructure | Active material volume fraction and radius, binder/additive volume ratio, compaction process | NMC | Minimizing specific resistance |
| Kabra et al. [133] | Stochastic 3D electrode generation, 3D physics-based pore scale simulation | linear regression, lasso regression, elasticnet, ridge regression, decision tree, adaboost, and gradient boost | Electrode mesostructure | Electrode composition (e.g. active material volume fraction), active material shape (e.g. equivalent radius), mean pore size, orientation | Graphite anode | Relationship between electrode mesostructures and physical properties |

multidisciplinary manner to address challenges in scalability, interpretability, and transferability of hybrid models. An essential requirement for this knowledge transfer and collaboration will include establishing knowledge-sharing platforms, workshops, and collaborations to disseminate findings and facilitate cross-disciplinary interactions in Lithium-ion battery hybrid modelling.

This field of research is rapidly evolving and advancing, and this roadmap should adapt to evolving research, technological advancements, and emerging challenges in battery technology, ensuring flexibility to incorporate novel methodologies and insights as they arise.

## 5. Future outlook and conclusions

More efficient deployment of LIBs is essential for a carbon emission-free future. For this to be achieved, more improvements must be made to develop and engineer high-performing LIBs. Employing digital tools for LIB research and development can accelerate the discovery of more effective battery designs by providing the opportunity to virtually test the impact of new design ideas on battery performance during its whole lifetime and under various working conditions. By evolving from simple empirical and ECMs to precise electrochemical models, simulations of LIBs have reached a high level of maturity. It is now possible to develop realistic 3D digital models of LIBs that consider the effect of degradation modes, heat generation, and material inhomogeneities and can closely imitate an actual battery's behavior. Such high-precision models can provide valuable information regarding how internal battery parameters are affected throughout a battery's life. However, the high computational cost of these models is the primary obstacle to their widespread use. Physics-informed machine learning has been proven to perform well as a surrogate for complicated physics-based battery models by reducing computation costs while maintaining accuracy. The application of physics-informed ML within the field of LIBs has primarily focused on developing fast models suitable for battery monitoring and state estimation during operation. It has also been proven that physics-informed ML surrogates can be used to achieve the optimal design leading to improved performance from pack to mesoscale level.

Despite this, some aspects of the current research can be improved to maximize the potential of hybrid methods. The models used in research for training dataset generation are not the most accurate and suffer from shortcomings. Integrating more precise multi-physics models with intensive details that simulate battery electrochemical reactions, thermal, aging, and mechanical behavior during the system's operation with ML algorithms can lead to more reliable results. In addition, large datasets of synthetic data are used to train ML algorithms to find the mapping between the LIB structure and property. Including the physics of the system more precisely by enforcing physical constraints to the loss

function can increase the reliability of the results by reducing the risk of producing physically unfeasible data when extrapolating beyond the training data [134]. Using a database of previous experiments or simulations of novel LIB structures can be useful for the model parameterization process and ML training [135]. Including experimental data in the training process of ML can increase the accuracy of the results by considering the effect of battery processes that might not be captured in the multi-physics model [136]. Also, when trying to find the optimal design of a battery component such as electrodes, it would be more accurate to extract the initial parameters of the multi-physics model from the performance curves of similar structures.

There are some challenges involved in developing a hybrid digital framework for LIB design. Development and parameterization of the multi-physics battery models are challenging due to the complexities involved in the system and large sets of required parameters. There are several coupled partial differential equations describing the behavior of the battery that must be solved simultaneously. It might be difficult to add all these equations to the loss function. Given that the challenges are addressed, combining three elements of high-fidelity multi-physics modeling, intelligent ML algorithms, and large experimental and simulation data can lead to developing a computationally efficient LIB simulation framework that can be used as a digital battery lab. Using this tool, electrode structures that satisfy different performance criteria simultaneously (e.g., high energy and power density, reduced lithium plating, and increased safety) can be obtained, leading to the development of the next generation of LIBs.

Verifying advanced digital LIB hybrid models through physical verification poses significant challenges due to the complexity and fidelity of digital designs. Recreating these digitally developed models in a laboratory setting can be difficult due to complexity of designs, high dimensionality and multivariate nature, resource and time constraints, accuracy and calibration challenges, and the dynamic and evolving nature of the LIB research and development field. To overcome these challenges, interdisciplinary collaborations involving experts in modelling, experimental analysis, and ML are essential. By combining aspects of hybrid modelling with targeted physical experiments can provide validation and refinement of digital results. Moreover, advancements in technology and innovative experimental techniques are continuously sought, and can prove to bridge the gap between digital models and physical verification in advanced LIB research. This procedure can be enhanced by collecting and sharing multiple datasets from various studies in a standard and interpretable manner, providing researchers with valuable information derived from both simulations and experiments.

With the need to electrify the energy sector with renewable energy to prevent climate change, batteries will play a significant role. The work presented here is of particular importance to the development of high-performance LIBs. By leveraging digital tools for LIB experimentation, it will allow research in the field of LIBs to progress faster than through traditional laboratory-based experimentation. At minimum, digital tools for battery experimentation can help guide further research in the laboratory to reduce development time. By expediting development of LIBs using digital tools, battery properties (e.g., power and energy) can be improved in a shorter time-frame. This is of interest for batteries used in transport applications, where battery size and mass are of importance.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

No data was used for the research described in the article.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rser.2024.114577.

## References

[1] Arun DM, Hamilton D, Krishna MN, Minakshi M. Design , development and thermal analysis of and stationary applications. Energies 2020;13.
[2] Morris M. COMPARISON OF RECHARGEABLE battery technologies Remote Ophthalmic system View project Upcycled/sustainable Robotics View project. November 2012, 2012.
[3] Zhang Z, Zhang SS. Challenges of key materials for rechargeable batteries. Green Energy Technol. 2015;172:1–24.
[4] Liang Y, et al. A review of rechargeable batteries for portable electronic devices. InfoMat 2019;1(1):6–32.
[5] Spitthoff L, Shearing PR, Burheim OS. Temperature, ageing and thermal management of lithium-ion batteries. Energies 2021;14:1248.
[6] Chu S, Majumdar A. Opportunities and challenges for a sustainable energy future. Nature 2012;488(7411):294–303.
[7] Chen T, et al. Applications of lithium-ion batteries in grid-scale energy storage systems. Trans Tianjin Univ 2020;26(3):208–17.
[8] Hossain Lipu MS, et al. Intelligent algorithms and control strategies for battery management system in electric vehicles: progress, challenges and future outlook. J Clean Prod 2021;292.
[9] Gao X, et al. Designed high-performance lithium-ion battery electrodes using a novel hybrid model-data driven approach. Energy Storage Mater 2021;36 (January):435–58.
[10] Fichtner M, et al. Rechargeable batteries of the future—the state of the art from a BATTERY 2030+ perspective. Adv Energy Mater 2022;12(17).
[11] Franco AA, et al. Boosting rechargeable batteries R&D by multiscale modeling: Myth or reality? Chem. Rev. 2019;119(7):4569–627.
[12] Advanced energy materials - 2022 - Zhang - digital twin enables Rational design of Ultrahigh-power lithium Ion Batteries (1).pdf. .
[13] Ramadesigan V, Northrop PWC, De S, Santhanagopalan S, Braatz RD, Subramanian VR. Modeling and simulation of lithium-ion batteries from a systems engineering perspective. J Electrochem Soc 2012;159(3):R31–45.
[14] Wang W, Wang J, Tian J, Lu J, Xiong R. Application of digital twin in smart battery management systems. Chinese J. Mech. Eng. (English Ed. 2021;34(1).
[15] VanDerHorn E, Mahadevan S. Digital twin: Generalization, characterization and implementation. Decis Support Syst 2021;145(February):113524.
[16] Qu X, Song Y, Liu D, Cui X, Peng Y. Lithium-ion battery performance degradation evaluation in dynamic operating conditions based on a digital twin model. Microelectron Reliab 2020;114(July).
[17] Panwar NG, Singh S, Garg A, Gupta AK, Gao L. Recent advancements in battery management system for Li-ion batteries of electric vehicles: future role of digital twin, Cyber-physical systems, battery Swapping technology, and Nondestructive testing. Energy Technol 2021;9(8):1–17.
[18] Sancarlos A, Cameron M, Abel A, Cueto E, Duval JL, Chinesta F. From ROM of Electrochemistry to AI-based battery digital and hybrid twin 2021;28(3).
[19] Tang X, Sun Y, Zhao Y, Pei W, Li N, Kong L. Digital twin based BESS state estimation and operating Opimization. 5th IEEE Conf. Energy Internet energy Syst. Integr. Energy Internet carbon neutrality. 2021. p. 3402–5. *EI2*.

[20] Wu B, Widanage WD, Yang S, Liu X. Battery digital twins: perspectives on the fusion of models, data and artificial intelligence for smart battery management systems. Energy 2020;1:100016.
[21] Ibrahim M, Rassölkin A, Vaimann T, Kallaste A. Overview on digital twin for Autonomous electrical vehicles Propulsion drive system. Sustain Times 2022;14 (2).
[22] Singh S, Weeber M, Birke KP. Advancing digital twin implementation: a toolbox for modelling and simulation. Procedia CIRP 2021;99:567–72.
[23] Park J, et al. Digital twin-driven all-solid-state battery: Unraveling the physical and electrochemical behaviors. Adv Energy Mater 2020;10(35):1–10.
[24] VanDerHorn E, Mahadevan S. Digital twin: Generalization, characterization and implementation. Decis Support Syst 2021;145:113524.
[25] Tran NT, Farrell T, Vilathgamuwa M, Choi SS, Li Y. A computationally efficient coupled electrochemical-thermal model for large format cylindrical lithium ion batteries. J Electrochem Soc 2019;166(13):A3059–71.
[26] Dao TS, Vyasarayani CP, McPhee J. Simplification and order reduction of lithium-ion battery model based on porous-electrode theory. J Power Sources 2012;198: 329–37.
[27] Nuroldayeva G, Serik Y, Adair D, Uzakbaiuly B, Bakenov Z. Review article state of health estimation methods for lithium-ion batteries, vol. 2023; 2023.
[28] Brosa Planella F, et al. A continuum of physics-based lithium-ion battery models reviewed. Prog. Energy 2022;4(4).
[29] Chen X, Liu X, Shen X, Zhang Q. Applying machine learning to rechargeable batteries: from the Microscale to the Macroscale. Angew. Chemie - Int. Ed. 2021; 60(46):24354–66.
[30] Duquesnoy M, Liu C, Dominguez DZ, Kumar V, Ayerbe E, Franco AA. Machine learning-assisted multi-objective optimization of battery manufacturing from synthetic data generated by physics-based simulations. Energy Storage Mater 2023;56:50–61.
[31] Liu K, Wang Y, Lai X. Data Science-based battery manufacturing management. Green Energy Technol.; 2022. p. 49–90.
[32] Liu X, et al. Bridging multiscale characterization technologies and digital modeling to evaluate lithium battery full lifecycle. Adv Energy Mater 2022;12 (33):1–25.
[33] Li G. Regulating mass transport behavior for high-performance lithium metal batteries and fast-charging lithium-ion batteries. Adv Energy Mater 2021;11(7): 1–14.
[34] O'Kane SEJ, et al. Lithium-ion battery degradation: how to model it. Phys Chem Chem Phys 2022;24(13):7909–22.
[35] Han X, et al. A review on the key issues of the lithium ion battery degradation among the whole life cycle. eTransportation 2019;1:100005.
[36] Zhang L, Lyu C, Wang L, Zheng J, Luo W, Ma K. Parallelized genetic identification of the thermal-electrochemical model for lithium-ion battery. Adv Mech Eng 2013;2013.
[37] Lawder MT, et al. Battery energy storage system (BESS) and battery management system (BMS) for grid-scale applications. Proc IEEE 2014;102(6):1014–30.
[38] Tran MK, Mevawala A, Panchal S, Raahemifar K, Fowler M, Fraser R. Effect of integrating the hysteresis component to the equivalent circuit model of Lithium-ion battery for dynamic and non-dynamic applications. J Energy Storage 2020;32 (May):101785.
[39] Lai X, et al. A comparative study of global optimization methods for parameter identification of different equivalent circuit models for Li-ion batteries. Electrochim Acta 2019;295:1057–66.
[40] Lai X, Zheng Y, Sun T. A comparative study of different equivalent circuit models for estimating state-of-charge of lithium-ion batteries. Electrochim Acta 2018; 259:566–77.
[41] Farmann A, Sauer DU. Comparative study of reduced order equivalent circuit models for on-board state-of-available-power prediction of lithium-ion batteries in electric vehicles. Appl Energy 2018;225(April):1102–22.
[42] Zhou W, Zheng Y, Pan Z, Lu Q. Review on the battery model and SOC estimation method. Processes 2021;9(9).
[43] Wang Z, Feng G, Zhen D, Gu F, Ball A. A review on online state of charge and state of health estimation for lithium-ion batteries in electric vehicles. Energy Rep 2021;7:5141–61.
[44] Kalogiannis T, et al. Comparative study on parameter identification methods for dual-polarization lithium-ion equivalent circuit model. Energies 2019;12(21): 1–37.
[45] Tran MK, et al. A comprehensive equivalent circuit model for lithium-ion batteries, incorporating the effects of state of health, state of charge, and temperature on model parameters. J Energy Storage 2021;43(September): 103252.
[46] Mousavi G SM, Nikdel M. Various battery models for various simulation studies and applications. Renew Sustain Energy Rev 2014;32:477–85.
[47] Huang K, Wang Y, Feng J. Research on equivalent circuit Model of Lithium-ion battery for electric vehicles. Proc. - 2020 3rd World Conf. Mech. Eng. Intell. Manuf. WCMEIM 2020:492–6.
[48] Nyman A, Zavalis TG, Elger R, Behm M, Lindbergh G. Analysis of the polarization in a Li-ion battery cell by Numerical simulations. J Electrochem Soc 2010;157 (11):A1236.
[49] Hossain E, Murtaugh D, Mody J, Faruque HMR, Sunny MSH, Mohammad N. A comprehensive review on second-life batteries: current state, manufacturing considerations, applications, impacts, Barriers potential solutions, Business strategies, and Policies. IEEE Access 2019;7(June):73215–52.
[50] Zhang Q, Shang Y, Li Y, Cui N, Duan B, Zhang C. A novel fractional variable-order equivalent circuit model and parameter identification of electric vehicle Li-ion batteries. ISA Trans 2020;97:448–57.
[51] Lai X, Wang S, Ma S, Xie J, Zheng Y. Parameter sensitivity analysis and simplification of equivalent circuit model for the state of charge of lithium-ion batteries. Electrochim Acta 2020;330:135239.
[52] Cho S, Jeong H, Han C, Jin S, Lim JH, Oh J. State-of-charge estimation for lithium-ion batteries under various operating conditions using an equivalent circuit model. Comput Chem Eng 2012;41:1–9.
[53] Fotouhi A, Auger DJ, Propp K, Longo S, Wild M. A review on electric vehicle battery modelling: from Lithium-ion toward Lithium-Sulphur. Renew Sustain Energy Rev 2016;56(April):1008–21.
[54] Zhang D, Popov BN, White RE. Modeling lithium intercalation of a single Spinel particle under Potentiodynamic control. J Electrochem Soc 2000;147(3):831.
[55] Guo M, Sikha G, White RE. Single-particle model for a lithium-ion cell: thermal behavior. J Electrochem Soc 2011;158(2):A122.
[56] Jokar A, Rajabloo B, Désilets M, Lacroix M. Review of simplified Pseudo-two-Dimensional models of lithium-ion batteries. J Power Sources 2016;327:44–55.
[57] Han X, Ouyang M, Lu L, Li J. Simplification of physics-based electrochemical model for lithium ion battery on electric vehicle. Part I: diffusion simplification and single particle model. J Power Sources 2015;278:802–13.
[58] Grandjean TRB, Li L, Odio MX, Widanage WD. Global sensitivity analysis of the single particle lithium-ion battery model with electrolyte. 2019 IEEE Veh. Power Propuls. Conf. VPPC 2019. Proc.; 2019.
[59] Li J, Lotfi N, Landers RG, Park J. A single particle model for lithium-ion batteries with electrolyte and stress-enhanced diffusion physics. J Electrochem Soc 2017; 164(4):A874–83.
[60] Lotfi N, Li J, Landers RG, Park J. Li-Ion battery state of health estimation based on an improved single particle model. Proc Am Control Conf 2017:86–91.
[61] Doyle M, Fuller TF, Newman J. Modeling of galvanostatic charge and discharge of the lithium/Polymer/Insertion cell. J Electrochem Soc 1993;140(6):1526–33.
[62] Torabi F, Ahmadi P. Simulation of battery systems: Fundamentals and applications. Simul. Batter. Syst. Fundam. Appl.; Jan. 2019. p. 1–409.
[63] Bizeray AM, Zhao S, Duncan SR, Howey DA. Lithium-ion battery thermal-electrochemical model-based state estimation using orthogonal collocation and a modified extended Kalman filter. J Power Sources 2015;296:400–12.
[64] Fuller TF, Doyle M, Newman J. Simulation and optimization of the dual lithium ion Insertion cell. J Electrochem Soc 1994;141(1):1–10.
[65] Gu WB, Wang CY. Thermal and electrochemical coupled modeling of a lithium-ion cell, in lithium batteries. ECS Proc. 2000;99–25(1):748–62.
[66] Zhao R, Liu J, Gu J. The effects of electrode thickness on the electrochemical and thermal characteristics of lithium ion battery. Appl Energy 2015;139:220–9.
[67] Panchal S, Mathew M, Fraser R, Fowler M. Electrochemical thermal modeling and experimental measurements of 18650 cylindrical lithium-ion battery during discharge cycle for an EV. Appl Therm Eng 2018;135(February):123–32.
[68] An Z, Jia L, Wei L, Dang C, Peng Q. Investigation on lithium-ion battery electrochemical and thermal characteristic based on electrochemical-thermal coupled model. Appl Therm Eng 2018;137(February):792–807.
[69] Wang Q, Jiang B, Li B, Yan Y. A critical review of thermal management models and solutions of lithium-ion batteries for the development of pure electric vehicles. Renew Sustain Energy Rev 2016;64:106–28.
[70] Ramadass P, Haran B, Gomadam PM, White R, Popov BN. Development of first principles capacity fade model for Li-ion cells. J Electrochem Soc 2004;151(2): A196.
[71] Zhang X, et al. A novel quantitative electrochemical aging model considering side reactions for lithium-ion batteries. Electrochim Acta 2020;343:136070.
[72] Edouard C, Petit M, Forgez C, Bernard J, Revel R. Parameter sensitivity analysis of a simplified electrochemical and thermal model for Li-ion batteries aging. J Power Sources 2016;325:482–94.
[73] Gao Y, et al. Health-aware Multiobjective optimal model for lithium-ion battery 2020;16(5):3417–29.
[74] Prada E, Di Domenico D, Creff Y, Bernard J, Sauvant-Moynot V, Huet F. A simplified electrochemical and thermal aging model of LiFePO 4 -graphite Li-ion batteries: power and capacity fade simulations. J Electrochem Soc 2013;160 (4):A616–28.
[75] Yang XG, Leng Y, Zhang G, Ge S, Wang CY. Modeling of lithium plating induced aging of lithium-ion batteries: Transition from linear to nonlinear aging. J Power Sources 2017;360:28–40.
[76] Lucu M, Martinez-Laserna E, Gandiaga I, Camblong H. A critical review on self-adaptive Li-ion battery ageing models. J Power Sources 2018;401(May):85–101.
[77] Schmalstieg J, Käbitz S, Ecker M, Sauer DU. A holistic aging model for Li (NiMnCo)O2 based 18650 lithium-ion batteries. J Power Sources 2014;257: 325–34.
[78] Redondo-Iglesias E, Venet P, Pelissier S. Modelling lithium-ion battery ageing in electric vehicle applications—calendar and cycling ageing combination effects. Batteries 2020;6(1):1–18.
[79] Liu K, Ashwin TR, Hu X, Lucu M, Widanage WD. An evaluation study of different modelling techniques for calendar ageing prediction of lithium-ion batteries. Renew Sustain Energy Rev 2020;131:110017.
[80] Christensen J, Newman J. A mathematical model of stress generation and fracture in lithium Manganese Oxide. J Electrochem Soc 2006;153(6):A1019.
[81] Duan X, Jiang W, Zou Y, Lei W, Ma Z. A coupled electrochemical–thermal–mechanical model for spiral-wound Li-ion batteries. J Mater Sci 2018;53(15):10987–1001.
[82] Ai W, Kraft L, Sturm J, Jossen A, Wu B. Electrochemical thermal-mechanical modelling of stress inhomogeneity in lithium-ion pouch cells. J Electrochem Soc 2020;167(1):013512.

[83] chun Yang S, Hua Y, Qiao D, bo Lian Y, wei Pan Y, ling He Y. A coupled electrochemical-thermal-mechanical degradation modelling approach for lifetime assessment of lithium-ion batteries. Electrochim Acta 2019;326:134928.
[84] Kim GH, Pesaran A, Spotnitz R. A three-dimensional thermal abuse model for lithium-ion cells. J Power Sources 2007;170(2):476–89.
[85] Christensen J, Albertus P, Cook D. A three-dimensional lithium-ion battery model that includes thermal, electrical and electrochemical behavior: I. Model description and validation. ECS Meet. Abstr. 2011;(28).
[86] Fang W, Ramadass P, Zhang Z. Study of internal short in a Li-ion cell-II. Numerical investigation using a 3D electrochemical-thermal model. J Power Sources 2014;248:1090–8.
[87] Yokoshima T, et al. Direct observation of internal state of thermal runaway in lithium ion battery during nail-penetration test. J Power Sources 2018;393 (April):67–74.
[88] Ghalkhani M, Bahiraei F, Nazri GA, Saif M. Electrochemical–thermal model of pouch-type lithium-ion batteries. Electrochim Acta 2017;247:569–87.
[89] Bahiraei F, Ghalkhani M, Fartaj A, Nazri GA. A pseudo 3D electrochemical-thermal modeling and analysis of a lithium-ion battery for electric vehicle thermal management applications. Appl Therm Eng 2017;125:904–18.
[90] Hein S, Feinauer J, Westhoff D, Manke I, Schmidt V, Latz A. Stochastic microstructure modeling and electrochemical simulation of lithium-ion cell anodes in 3D. J Power Sources 2016;336:161–71.
[91] Singh S, Weeber M, Birke KP. Implementation of battery digital twin: approach, functionalities and benefits. Batteries 2021;7(4):1–21.
[92] Sulzer V, Marquis SG, Timms R, Robinson M, Chapman SJ. Python battery mathematical modelling (PyBaMM). J. Open Res. Softw. 2021;9:1–8.
[93] Cai L, White RE. Mathematical modeling of a lithium ion battery with thermal effects in COMSOL Inc. Multiphysics (MP) software. J Power Sources 2011;196 (14):5985–9.
[94] Santhanagopalan S, Long C, White RE. Mathematical modeling of lithium ion batteries. ECS Trans 2008;16(13):81–90.
[95] Torchio M, Magni L, Gopaluni RB, Braatz RD, Raimondo DM. LIONSIMBA: a Matlab framework based on a finite volume model suitable for Li-ion battery design, simulation, and control. J Electrochem Soc 2016;163(7):A1192–205.
[96] Gao T, Lu W. Machine learning toward advanced energy storage devices and systems. iScience 2021;24(1):101936.
[97] Wahl MS, Spitthoff L, Muri HI, Jinasena A, Burheim OS, Lamb JJ. The importance of Optical Fibres for internal temperature sensing in lithium-ion batteries during operation. Energies 2021;14(12):3617.
[98] Jinasena A, et al. Online internal temperature sensors in lithium-ion batteries: state-of-the-art and future trends. Front. Chem. Eng. 2022;4(February):1–22.
[99] Gu GH, Noh J, Kim I, Jung Y. Machine learning for renewable energy materials. J Mater Chem A 2019;7(29):17096–117.
[100] Wei Z, He Q, Zhao Y. Machine learning for battery research. J Power Sources 2022;549(July):232125.
[101] Zhang L, et al. The machine learning in lithium-ion batteries: a review. Eng Anal Bound Elem 2022;141(March):1–16.
[102] Wu B, Widanage WD, Yang S, Liu X. Battery digital twins: perspectives on the fusion of models, data and artificial intelligence for smart battery management systems. Energy 2020;1:100016.
[103] Espedal IB, Jinasena A, Burheim OS, Lamb JJ. Current trends for state-of-charge (SoC) estimation in lithium-ion battery electric vehicles. Energies 2021;14(11).
[104] Lombardo T, et al. Artificial intelligence applied to battery research: Hype or reality? Chem. Rev. 2021.
[105] Allam O, Cho BW, Kim KC, Jang SS. Application of DFT-based machine learning for developing molecular electrode materials in Li-ion batteries. RSC Adv 2018;8 (69):39414–20.
[106] Pattavathi B, Surendran V, Palani S, Shaijumon MM. Artificial neural network-enabled approaches toward mass balancing and cell optimization of lithium dual ion batteries. J Energy Storage 2023;68(February):107878.
[107] Eddahech A, Briat O, Bertrand N, Delétage JY, Vinassa JM. Behavior and state-of-health monitoring of Li-ion batteries using impedance spectroscopy and recurrent neural networks. Int J Electr Power Energy Syst 2012;42(1):487–94.
[108] Lipu MSH, Hannan MA, Hussain A, Saad MHM, Ayob A, Muttaqi KM. Lithium-ion battery state of charge estimation method using optimized deep recurrent neural network algorithm. 2019 IEEE Ind. Appl. Soc. Annu. Meet. IAS 2019. 2019. p. 1–9.
[109] Xu Z, Wang J, Fan Q, Lund PD, Hong J. Improving the state of charge estimation of reused lithium-ion batteries by abating hysteresis using machine learning technique. J Energy Storage 2020;32(2).
[110] Ma Y, Shan C, Gao J, Chen H. A novel method for state of health estimation of lithium-ion batteries based on improved LSTM and health indicators extraction. Energy 2022;251.
[111] Zhang Y, Xiong R, He H, Pecht MG. Long short-term memory recurrent neural network for remaining useful life prediction of lithium-ion batteries. IEEE Trans Veh Technol 2018;67(7):5695–705.
[112] Richardson RR, Birkl CR, Osborne MA, Howey DA. Gaussian process regression for in Situ capacity estimation of lithium-ion batteries. IEEE Trans. Ind. Informatics 2019;15(1):127–38.
[113] Sahinoglu GO, Pajovic M, Sahinoglu Z, Wang Y, Orlik PV, Wada T. Battery state-of-charge estimation based on Regular/recurrent Gaussian process regression. IEEE Trans Ind Electron 2018;65(5):4311–21.
[114] Attarian Shandiz M, Gauvin R. Application of machine learning methods for the prediction of crystal system of cathode materials in lithium-ion batteries. Comput Mater Sci 2016;117:270–8.
[115] Berecibar M, et al. Online state of health estimation on NMC cells based on predictive analytics. J Power Sources 2016;320:239–50.
[116] Zhu S, Zhao N, Sha J. Predicting battery life with early cyclic data by machine learning. Energy Storage 2019;1(6):1–5.
[117] Yang F, Wang D, Xu F, Huang Z, Tsui KL. Lifespan prediction of lithium-ion batteries based on various extracted features and gradient boosting regression tree model. J Power Sources 2020;476(May).
[118] Li Y, et al. Random forest regression for online capacity estimation of lithium-ion batteries. Appl Energy 2018;232(October):197–210.
[119] Liu K, Hu X, Zhou H, Tong L, Widanage WD, Marco J. Feature Analyses and modeling of lithium-ion battery manufacturing based on random forest classification. IEEE/ASME Trans. Mechatronics 2021;26(6):2944–55.
[120] Dawson-Elli N, Subramanian VR, Schwartz DT, Beck DAC. The role of data science in Numerical modeling of lithium ion batteries. 2019.
[121] Dawson-Elli N, Lee SB, Pathak M, Mitra K, Subramanian VR. Data science approaches for electrochemical engineers: an introduction through surrogate model development for lithium-ion batteries. J Electrochem Soc 2018;165(2): A1–15.
[122] Li W, et al. Physics-informed neural networks for electrode-level state estimation in lithium-ion batteries. J Power Sources 2021;506(June).
[123] Tu H, Moura S, Wang Y, Fang H. Integrating physics-based modeling with machine learning for lithium-ion batteries. SSRN Electron J 2022.
[124] Feng F, et al. Co-estimation of lithium-ion battery state of charge and state of temperature based on a hybrid electrochemical-thermal-neural-network model. J Power Sources 2020;455(March):227935.
[125] Chun H, Kim J, Yu J, Han S. Real-time parameter estimation of an electrochemical lithium-ion battery model using a long short-term memory network. IEEE Access 2020;8:81789–99.
[126] Wu B, Han S, Shin KG, Lu W. Application of artificial neural networks in design of lithium-ion batteries. J Power Sources 2018;395:128–36.
[127] Gao T, Lu W. Physical model and machine learning enabled electrolyte channel design for fast charging. J Electrochem Soc 2020;167(11):110519.
[128] Deng C, Lu W. Geometry optimization of porous electrode for lithium-ion batteries. ECS Meet. Abstr. 2020;(4).
[129] Advanced energy materials - 2022 - Sui - bio-inspired computational design of vascularized electrodes for high-performance.pdf.
[130] Yamanaka T, Takagishi Y, Yamaue T. A framework for optimal safety Li-ion batteries design using physics-based models and machine learning approaches. J Electrochem Soc Jun. 2020;167(10):100516.
[131] Li A, et al. Integration of computational fluid dynamics and artificial neural network for optimization design of battery thermal management system. Batteries Jul. 2022;8(7):69.
[132] Takagishi Y, Yamanaka T, Yamaue T. Machine learning approaches for designing mesoscale structure of li-ion battery electrodes. Batteries 2019;5(3).
[133] Kabra V, Birn B, Kamboj I, Augustyn V, Mukherjee PP. Mesoscale machine learning analytics for electrode property estimation. J Phys Chem C 2022;126 (34):14413–29.
[134] Aykol M, et al. Perspective—combining physics and machine learning to predict battery lifetime. J Electrochem Soc 2021;168(3):030525.
[135] Gao X, et al. Designed high-performance lithium-ion battery electrodes using a novel hybrid model-data driven approach. Energy Storage Mater 2021;36 (October 2020):435–58.
[136] Vegge T, Tarascon JM, Edström K. Toward better and smarter batteries by combining AI with Multisensory and self-Healing approaches. Adv Energy Mater 2021;11(23).
[137] Ren D, et al. Systematic optimization of battery materials: key parameter optimization for the scalable Synthesis of uniform, high-energy, and high stability LiNi0.6Mn0.2Co0.2O2 cathode material for lithium-ion batteries. ACS Appl Mater Interfaces 2017;9(41):35811–9.
[138] Dotoli M, et al. Li-ion battery systems. 2022. p. 1–18.
[139] Nitta N, Wu F, Lee JT, Yushin G. Li-ion battery materials: Present and future. Mater Today 2015;18(5):252–64.
[140] Westhoff D, Manke I, Schmidt V. Generation of virtual lithium-ion battery electrode microstructures based on spatial stochastic modeling. Comput Mater Sci 2018;151(April):53–64.
[141] Zhu J, Wierzbicki T, Li W. A review of safety-focused mechanical modeling of commercial lithium-ion batteries. J Power Sources 2018;378:153–68.
[142] Lee H, et al. Understanding the effects of diffusion coefficient and exchange current density on the electrochemical model of lithium-ion batteries. Curr Opin Electrochem 2022;34:100986.
[143] wei Pan Y, et al. A computational multi-node electro-thermal model for large prismatic lithium-ion batteries. J Power Sources 2020;459(March):228070.
[144] Saw LH, Ye Y, Tay AAO, Chong WT, Kuan SH, Yew MC. Computational fluid dynamic and thermal analysis of Lithium-ion battery pack with air cooling. Appl Energy 2016;177:783–92.
[145] Wu H, Cui Y. Designing nanostructured Si anodes for high energy. Nano Today 2012;7:414–29.
[146] Liao Z, Zhang S, Li K, Zhang G, Habetler TG. A survey of methods for monitoring and detecting thermal runaway of lithium-ion batteries. J Power Sources 2019; 436:226879.