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Module-Level Modelling Approach for a Cloud-based Digital Twin Platform for Li-Ion Batteries

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Abstract— The pursue of the new increasingly intelligent, and heavier state estimation algorithms requires a significant amount of data and computing power, which may challenge their deployment in current BMS solutions. To address that issue, this paper proposes a cloud-based Digital Twin Platform to extend computing power and data storage capacity. This tool aims to contain the integration of models to analyse thermo-electric and ageing aspects of a LIB, based on experimental operation data by comparative analysis. Based on well-known cell-level modelling techniques, a module-level modelling approach is proposed and an experimental validation platform is suggested.

Keywords—Digital Twin, Cloud computing, Battery models, State of Charge

I. INTRODUCTION

In the path towards the reduction of carbon emissions, electric vehicles and renewable energy systems are key technologies. Both are typically based on Lithium-ion batteries (LIB), in virtue of making the most of the energy of each application [1]. However, battery cost is still high and their lifetime is finite, as this technology degrades over time and cycling, thus suffering a drop in performance. Accurate monitoring and control of LIBs is important to avoid problems related to safety, reliability, durability and cost of LIBs [2]. Nevertheless, the estimation and prediction of LIB performance in real operating conditions is still a challenge, due to the highly non-linear and coupled phenomena taking place on battery behaviour [3].

Since battery internal states are hardly measurable, and often based on offline invasive methods, it is necessary to develop methods oriented to estimate such instantaneous internal states. State of Charge (SoC), State of Power (SoP) and State of Health (SoH) are some of the typical key X states (SoX) that are tracked in the battery BMS. Additionally, ageing models are developed for the estimation of the Remaining Useful Lifetime (RUL).

The information provided by these states allows the design of operational strategies, the diagnosis of error conditions, thermal management, or optimal control of loads to prolong battery lifetime. However, the models employed to estimate these states typically imply a large amount of training data and most advanced algorithms require a computational power that typical industrial BMS lack [4].

With batteries becoming increasingly connected due to the use of Internet of Things (IoT) technologies, there is the possibility of collecting real operation data once the batteries are deployed. In addition, with the availability of that large amounts of data plus cloud-based models, the Digital Twin

(DT) concept has emerged [5]. In a battery DT, there is a close interaction between the physical entity, its virtual counterpart, and the aggregation of in-field data over their entire lifetime. Creating a battery DT environment in which the models, data and Machine Learning (ML) tools are integrated, makes possible to have a cloud BMS (cBMS) with an enhanced intelligence. This enables the application of key communication and networking technologies such as virtualisation, service-oriented architecture, real-time monitoring and opens up the potential of longer LIBs lifetime, increased reliability and enhanced safety.

With the final purpose of developing a battery DT, this work begins introducing the principles of operation of the cBMS (Section 1). Continuing with the description of the different battery models considered for the design of the cloud-based simulation platform (Section 2). The target cloud platform and the preliminary validation plan of the DT Platform Models are then presented (Section 3) and finally, the main conclusions and future work are highlighted.

II. BATTERY IN THE CLOUD

The different algorithms that monitor and control the LIBs are usually implemented in the BMS. State of the art BMS technologies are typically based on two main elements: i) a BMS-slave containing an Analog Front-End (AFE) which is responsible for monitoring the LIBs; and ii) a BMS-master which contains more advanced safety and diagnostic functions that require more computational power [6]. Some of the most important functions of the BMS are the estimation of the SoC and SoH. These states provide essential information about the energy available on the LIB and can be used for the design of operating strategies or maintenance and thereby increase the lifetime of the battery.

Among the different estimation algorithms [7]–[10], open-loop SoC algorithms (e.g. Coulomb counting or the Open Circuit Voltage method) require small computational power and are easy to implement in LIB onboard BMSs. However, the more accurate and robust estimation algorithms (e.g. based on Kalman Filters or ML) require higher computational power and can be challenging to implement them in onboard BMSs. In addition, these advanced algorithms are often based on historical data and therefore also require a significantly large database. Compared to SoC estimation, SoH estimation of LIBs is a more complex exercise due to multiple and non-linear degradation mechanisms typically taking place on LIBs [11], [12].

To overcome these challenges, the required performance of the BMS can be increased by implementing it together with cloud computing and IoT-based technology. Data from LIBs can be measured and transmitted to the cloud with IoT

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devices, then filtered and stored in a single database on the cloud platform (and later described in Fig. 3 and Fig. 4). This database can then be used to create the DT of the LIB.

Two of the main advantages of implementing the cBMS of the LIBs in the Cloud environment are, as mentioned above, the increase of computing power and the exponential increase in the capacity to store the data of the entire battery life. With this computational capacity, continuous monitoring is possible with the different state estimation algorithms. In addition, it allows predictions of LIB life prognosis by using new and more complex methods for RUL prediction [13], [14]. On the other hand, by being able to track historical LIB data from multiple energy storage systems deployed in different applications, anomalies in LIB operation can be detected. By predicting and detecting faults, the safety and reliability of the entire LIB system can be improved. That historical data can also be used to analyse different operating scenarios and thus improve and optimise the design of the battery system.

The battery DT can estimate and predict the different SoX of the LIBs thanks to the data obtained from the sensors and the advanced algorithms in the Cloud. However, in order to increase the reliability and safety of the system, some minimal functionalities are usually implemented in parallel in the onboard BMS. At the same time, a more advanced version of the algorithm runs in the Cloud providing a higher estimation accuracy.

III. PROPOSED CELL-LEVEL BATTERY MODELS

Concerning issues of performance and lifetime prediction of LIBs, models of different nature are often used. These typically describe the voltage response to a current load, the thermal performance and the evolution of capacity/resistance over the lifetime of the cells. There are currently a diversity of approaches in each type of models, and in the way they are integrated.

A. Electric Model

Batteries are typically modelled according to different physical phenomena [3], being Equivalent Circuit Models (ECM) one of the most common methods for battery electrical modelling. ECM uses electrical elements such as resistors and capacitors, as well as an Open Circuit Voltage (OCV) versus SoC profiles to replicate the voltage response of a battery. These are lighter than electrochemical models and depending on the specific battery chemistry and modelling accuracy desired, a different number of RC blocks can be used. Also hysteresis and constant phase elements are usually added.

Their level of complexity usually depends on the number of resistance-capacitor (RC) pairs they have. In this work, an ECM with an RC phase is chosen, which also considers the battery hysteresis. It has been chosen for its balance between accuracy and complexity versus computational cost. Fig. 1 describes the ECM to be implemented in the Digital Twin Simulation Platform (DTSP).

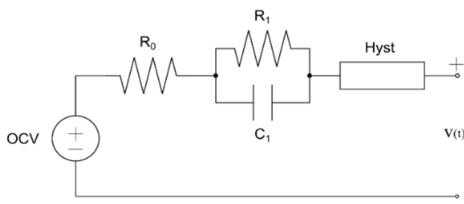


Fig. 1. Digital Twin Electric Equivalent Circuit Model.

The different parameters of the model are influenced by the temperature, the SoC and the SoH of the LIB. These parameters are obtained by different laboratory test such as Electrochemical Impedance Spectroscopy (EIS) or OCV vs SoC Test. Then, they are described by a lookup table and the model updates the value of the parameters at each step time.

The resistance in series (R_0) represents the energy that is dissipated by the internal resistance of the cell in the heat form. This element is usually a function of the SoC and is always dependent on the cell internal temperature.

$$v_{R_0}(k) = R_0 i(k) \quad (1)$$

The current flow through the R_1 is used to calculate the diffusion current of the cell. Then, the diffusion state ($i_{R_1}(k)$) is estimated by (2).

$$i_{R_1}(k+1) = \exp\left(\frac{-\Delta t}{R_1 C_1}\right) i_{R_1}(k) + \left(1 - \exp\left(\frac{-\Delta t}{R_1 C_1}\right)\right) i(k) \quad (2)$$

where, Δt is the time interval between the current k and the previous k values, R_1 and C_1 are the resistor and capacitor values in the ECM RC phase, $i_{R_1}(k)$ is the diffusion current through the R_1 resistor at time k and $i(k)$ is the current through the cell at time k .

The element labelled as "Hyst" in Fig. 1 represents the non-linear hysteresis of the cell. The hysteresis in the cell is described by the hysteresis state $h(k)$, which only changes as the cell SoC does. The hysteresis voltage is modelled by (3).

$$h(k+1) = \exp\left(-\left|\frac{\eta(k)i(k)\gamma\Delta t}{Q}\right|\right) h(k) - \left(1 - \exp\left(-\left|\frac{\eta(k)i(k)\gamma\Delta t}{Q}\right|\right)\right) \text{sgn}(i(k)) \quad (3)$$

where, $\eta(k)$ is cell coulombic efficiency, $i(k)$ is the current through the cell at time k , γ is a positive constant that refines the decay rate, Δt is the time interval between the current k and the previous k ($k-1$), Q is the current cell capacity, $h(k)$ is the hysteresis voltage and $\text{sgn}(i(k))$ forces the equation to be stable for both charging and discharging and represents the instantaneous drop of the hysteresis voltage.

The output equation of the model takes into account all the phenomena described above. The equation is defined in (4).

$$v(k) = OCV(k) + h(k) - R_1 i_{R_1}(k) - R_0 i(k) \quad (4)$$

For the estimation of the SoC of the LIB a SPKF based estimator was implemented according to the approach implemented by Dr. Gregory L. Plett [15]. It has a prediction sub step and a correction sub step that correct predictions to produce a state estimate together with their confidence limits in each measurement interval. More detailed information can be found in [15], [16].

B. Thermal Model

Thermal models are used to describe the thermal gradient of LIBs. These can be classified into two main groups, namely: i) Numerical Distributed Models using Computational Fluid Dynamics (CFD) methods and ii) Analytical Lumped Models. The former are generally used in

the battery design phase, while lumped models are lighter, being simplifications of heat distribution based on equivalent circuits.

The chosen and developed thermal lumped model is described in Fig. 2. The electrical circuit is an analogue to the heat generation, storage and transfer. It contains a series of data obtained in laboratory tests (e.g. Open Circuit Potentiometry (OCP)) stored in a lookup table. These parameters are adjusted at each time step for the estimation of the temperature at different points of the battery.

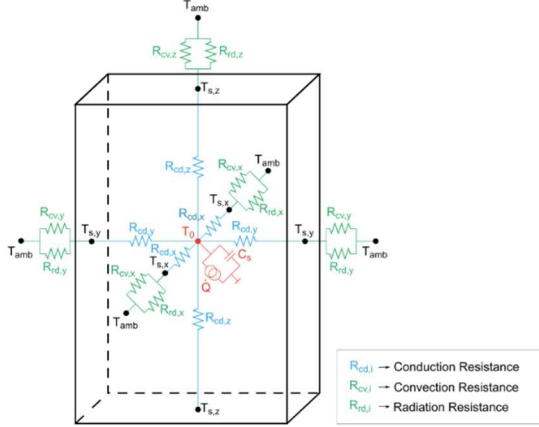


Fig. 2. Digital Twin Thermal Lumped Model.

The model is implemented in three dimensions. First, the heat generated by each cell (\dot{Q}) and the accumulated heat (\dot{C}_s) are calculated. In addition, the heat transferred to the cell surface by conduction ($Q_{cd,i}$) is calculated in all three dimensions. This heat transferred to the cell surface is then dissipated by convection ($Q_{cv,i}$) and radiation ($Q_{rd,i}$), also in all three dimensions. This heat power is calculated with the resistance corresponding to each of the cell geometries. The equations describing each of the thermal phenomena are described as:

$$q_{accu} = q_{gen} - q_{cond} \quad (5)$$

$$q_{cond,i} = q_{conv,i} + q_{rad,i} \quad (6)$$

where, q_{accu} is the heat accumulated between the current k and the previous $k-1$, q_{gen} is the heat generated by the current flowing through the cell, q_{cond} is the heat transferred by conduction from the centre to the surfaces of the cell and q_{conv} and q_{rad} is this conductive heat dissipation via convection and radiation. The index i represents each of the three dimensions through which the heat is transferred.

The thermodynamic energy balance for Li-ion batteries has been discussed in detail by Bernardi et al [17]. In this work, a simplified form of the heat generation equation presented by Nieto et al. [18] is used. It considers both the irreversible heat generated as Joule losses and the reversible heat generated by the cell.

$$\begin{aligned} q_{gen} &= I(V - U^{avg}) + IT \frac{dU^{avg}}{dT} \\ &= I^2 \cdot R_0 + I \cdot T \cdot EHC \end{aligned} \quad (7)$$

where, I is the current through the cell in Amperes; V is the terminal voltage of the cell in Volts; U^{avg} is the average OCV in Volts; T is the temperature of the cell in degrees Celsius

($^{\circ}\text{C}$) and dU^{avg}/dT is the Entropic Heat Coefficient (EHC) in (Volts/ $^{\circ}\text{C}$). The EHC must be measured in the laboratory as well as the Internal Resistance (R_0).

C. Ageing Model

Finally, battery ageing models are used to make RUL predictions. There are physics-based ageing models, data-driven approaches and semi-empirical models [13]. With the advance of technologies such as the IoT or Big Data (BD) and cloud-based computing, data-driven models are emerging as a promising candidate for RUL prediction [13].

In a recent review of data-driven aging models employed for lithium-ion battery ageing prediction, the Gaussian Process (GP) method was identified as the most promising candidate [4]. In fact, beyond their ability to make relatively robust probabilistic predictions, these models have the advantage of being non-parametric. Therefore, their complexity depends on the volume of contained training data. However, creating such a large training database is time- and cost-intensive. For this reason, it has been sought a model capable of learning based on the operating data once the battery is deployed, i.e. the GP.

The decrease of the SoH of the cells is progressive whether the cell is in operation (cycling ageing) or by the passage of time (calendar ageing). For this reason, it is relevant to model both modes of operation of the cells. The implemented GP-based ageing model was composed of both a calendar- and cycle-ageing components. Further details on the implemented models can be found in [19], [20].

IV. PROPOSED CLOUD PLATFORM AND EXPECTED PRELIMINARY VALIDATION RESULTS

A. Cell level Model Integration

The models previously presented are integrated in order to develop a DTSP based on cloud computing. This platform is destined to be the digital replica of the LIB, where different battery states can be estimated (SoX) to later enable a variety of Digital Services and, thereby, optimise battery operation through its entire lifecycle. In a first stage, different characterisation tests at Beginning of Life (BoL) will be carried out, in a second stage the battery will be degraded with a static profile. Periodically, Check-Ups (CU) will be performed in order to get the different model parameters at each SoH. The cycling tests will be used to parametrise both the electrical and the thermal model, and in turn, the CUs will serve to validate the ageing model. In addition, dynamic laboratory tests will be used to mimic real battery operating conditions in order to validate the electric and thermal models.

Each model's parameters at each activation time step are chosen according to the feedback from other models as shown in Fig. 3. The battery models will use the current data measured by the sensors together with the historical data stored in the cloud. Furthermore, additional data obtained in other applications will be aggregated, which can later be used for re-training the models in the DT. Thereby, the DT platform being developed not only integrates the data gathered on a single battery but will also allow integrating and learning from the operation of multiple batteries on a fleet.

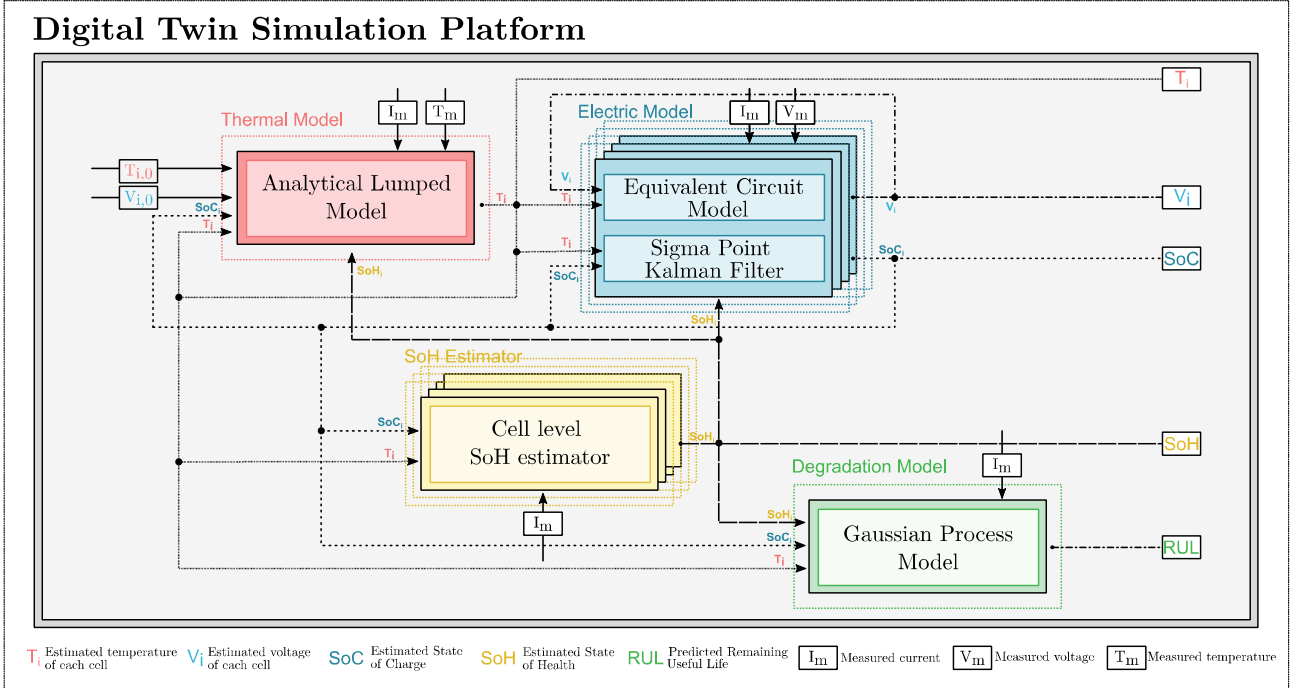


Fig. 3. Elements of a Digital Twin Battery

The implementation of these models at cell level is widespread in the literature. For example, the electrical model can be found in the work of Dr. Plett [16] in which a Sigma Point Kalman Filter (SPKF) is used to estimate the SoC of the cell. On the other hand, Nieto et al. [18] developed a Lumped thermal model. Also, the GF degradation model is used by Lucu et al. in [21]. In addition, studies have been carried out in which two or all three types of models have been integrated for the simulation of LIBs. Looking at some examples of the Electro-Thermal Aging Models, Shen et al. [22] developed a model to estimate the SoC of the cell, the internal cell temperature and the battery lifetime. The impact of various factors such as C-rate of charge and discharge, temperature, maximum discharge current and DoD, cycle time and their effects on the loss of battery cell capacity were investigated and studied. The model provided a battery terminal voltage, estimated SOC, temperature and capacity fading simultaneously through the evaluation of the input current. Mohajer et al. [23] proposed a model for the optimisation of the fast charge profile and a model-based design of an intelligent charge controller. On the other hand, Mesbahi et al. [24] designed a simple and sufficiently representative model of the physical phenomena occurring in a battery cell. They based the model on an equivalent circuit model coupled to a thermal circuit and a semi-empirical aging equation with an acceptable relative error of less than 1%, 4% and 2%, respectively.

All these developments, as well as the vast majority of those found in the literature, are designed and validated at cell level. Nevertheless, the actual outcome of a DTSP lies on its capability to model the LIB performance at the module level. The literature describing methods to extrapolate module level performance are scarce and most estimate the module states without considering the individual state of the cells. Such an approach may be valid under very specific conditions but can still lead to a significant inaccuracy when estimating and predicting the electric and thermal performance of certain module constructions. Aiming at overcoming such limitations,

the following section describes the proposed module level modelling approach.

B. Proposed Module Level Modelling Approach

A module is a package or array of cells in series or parallel connection, but due to unbalances, cell-to-cell variations and inhomogeneous operating conditions its final useful energy rarely is simply the sum of that of the individual cells. Therefore, a module-level extrapolation should be made to consider these variations caused by the cell-to-cell inhomogeneity or operating characteristics of the complete module [25].

Among the main sources of inhomogeneities at module-level battery performance, the following can be highlighted: i) cell-to-cell manufacturing variability, typically leading to heterogeneous capacity and internal resistance values; ii) inhomogeneous temperature distribution inside the module during operation or as a consequence of heterogeneous battery ageing; and iii) unbalanced battery operation, as a consequence of local current gradients or uneven battery consumption of the associated electronics (typically the BMS). For these reasons, the SoX of each cell needs to be accordingly estimated and then the equivalent response of all cells should be estimated.

First, it must be considered that not all models have the same dynamics, so they are not all necessarily executed at the same time. For example, the dynamics of the electric model is faster than those of the thermal model. Therefore, the electrical model will be implemented at each time step while the thermal model updates its estimates in a longer period of time. The same applies to the SoH estimator and the ageing model, as the degradation of the cells is considerably slower. Thus, electrical and thermal dynamics could be defined as fast dynamics and ageing as slow dynamics in a LIB.

Starting from an equilibrium condition with the cells at a defined SoH, there is no temperature gradient throughout the module. The BMS is responsible for measuring some of the

variables such as the voltage at the terminals of each cell or the temperature at specific points of the module and these are used as inputs for the DTSP models. Below, the method for estimating the SoX of each cell composing a LIB module is presented:

The thermal model is implemented in a first step at module level, considering all the cells, as the heat transferred between them needs to be considered at every moment. To estimate the temperature distribution within the module, the common points of the thermal equivalent circuits of the cells are joined according to the module topology and a meshed circuit is created. This implies that the operations to calculate the energy balance are multiplied by the number of cells. With this information, the equivalent temperature of all surfaces and core temperature of each cell are obtained. These are used to decide the equivalent temperature of each cell, which are referred as T_i . In addition, the model compares the estimates with the information obtained by the BMS from the thermocouples measurements. The module-level thermal model uses the updated information of the voltage and SoC (information estimated by the electrical model) and the SoH of each cell (generated by the SoH estimator).

The equivalent cell temperatures are used as input for the cell-level electric models. These temperatures are used to obtain the parameters of the electrical model together with the SoH and the operating current. The cell-level electrical model consists of an ECM and a SPKF, and it is implemented for each cell and co-simulated. Thus resulting in voltages and SoC calculations for all the cells in the module, which are referred as V_i and SoC_i . In cases in which temperature distributions and cell-to-cell electric parameter variations are low, the co-simulation of the electric model can be simplified into single or few cells simulation (considering averaged parameters) thus also reducing the computational burden at a reduced accuracy loss. Once the results from the electric models co-simulation are obtained, results are extrapolated to the module level by taking into account some previously defined criteria for the estimation of the Equivalent Module Voltage (EMV). This EMV is then used to estimate the equivalent SoC of the complete module (linked to the module series-parallel cell configuration).

At certain intervals (e.g. at defined Ah-throughput intervals or after specific periods of time), the SoH estimator has to be implemented, which updates the SoH information of each cell for the electrical model and the thermal model. This estimator uses the operating data of each cell to make the corresponding SOH estimations for each of the cells composing the module. In addition, periodically the GP model will also be executed with the purpose of obtaining new battery ageing predictions. This model collects the operation information from the LIB and then is trained together with the historical data from the database. As a result, the model predicts the ageing trend corresponding to each of the cells in the module, thus allowing to identify any potential cell-to-cell variations on their ageing behaviour.

Once the state of the cells is known, the module level characteristics are estimated. At this point, the estimates made by the three models (with variations and unbalances) and the topology will be considered to calculate the equivalent V, I and T of the module. Furthermore, the DTSP will provide a clearer representation of the temperature distribution at a great amount of points within the module, which is not typically affordable as LIB modules usually have a reduced number of

temperature sensors. In addition, this platform enables more accurate estimation of the SoC of each of the cells in the module. This, along with the temperature distribution can lead to more accurate SoH and RUL estimates.

C. Proposed Validation Platform

To implement this methodology, the proposed hardware is presented in Fig. 4.

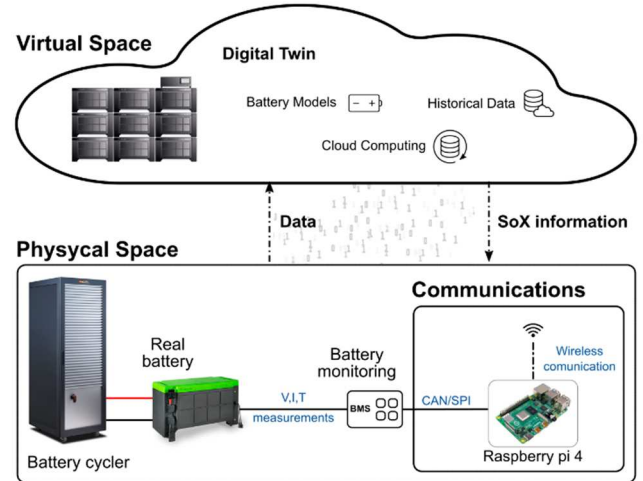


Fig. 4. Schematic diagram of the proposed DTSP validation platform.

The purpose is to build a battery prototype to validate the monitoring functionalities of the BMS in the cloud. The prototype will consist of 15 Lithium Iron Phosphate (LFP) cells of 3.2 V and 280 Ah connected in series. It is intended to parameterise and apply load profiles for its validation. A Digatron BNT 50-100-16(12) BDBT ME cycler with 50 V and 100 A test circuits will be used for this purpose, and the ambient temperature is controlled with a climatic chamber from the manufacturer CTS. The voltage and temperature of the twelve cells are measured and transmitted to the cloud.

This module is connected to a BMS developed by Ikerlan which takes care of functions such as measuring voltages and temperatures or the implementation of simpler algorithms. This BMS exchanges information with a Raspberry Pi 4 which is responsible for uploading all the necessary data to the cloud where the DTSP (with the LIB models) and the database are located. For the design of the models at the module level, it is intended to compare the results obtained by taking the module as a single unit and by implementing the models obtained at the cell level in each of the cells that constitute the module.

The electrical and thermal models which are equivalent circuits are models with a small complexity. The thermal Lumped model together with the ECM with the SPKF could be implemented locally in the battery BMS without major problems at the cell level. In case of considering the module as a single unit, no problems are foreseen for the implementation of these models either. However, as it is intended to implement the electrical model simultaneously to each cell, the BMS could have problems performing the on-board operations. In addition, the iterations to calculate the heat balance of the Lumped model will also need considerable computing power to work in real time. Nonetheless, this issue would not necessarily be a problem considering cloud computing systems.

The degradation model is non-parametric, which means that the size of this model increases when the training data

increases. This means that the larger this database is, the more computational power is required to implement the model. Furthermore, this is directly related to the memory storage capacity that the model will require to store all this historical cell data. These power and memory requirements may be critical from the perspective of implementing the model on the local battery system hardware. However, it would also not be a problem with cloud computing technology. Furthermore, one of the advantages of the DT is the connectivity so that it is also possible to save information from other batteries and complete the knowledge of the model. All of the above applies to the model at the cell level as well as at the module level.

V. CONCLUSIONS AND FUTURE WORK

Current LIB models most widely available in the literature typically target cell-level performance evaluation and simulation. Nevertheless, cell-to-cell variability and inhomogeneous operating conditions at the module level may actually imply significant performance and ageing deviations among the cells constituting a specific LIB module. This paper presents a DTSP framework consisting of electrical, thermal and ageing models of the LIB targeting their ultimate validation with experimental data obtained for realistic operating conditions. Starting from well-known cell level modelling techniques, a module level modelling approach is proposed. Additionally, the conceived validation platform was also presented, aiming to prove the performance of the models to be implemented. The strong coupling between the three models included is expected to ultimately impact on the reliability of the RUL predictions to be obtained. Thereby, the presented DTSP framework is expected to constitute a thorough yet computationally efficient module-level modelling approach, covering both the model architecture and the proposed validation platform.

The implementation process of the module-level models here described is still ongoing. Results from the modelling approach and the validation results will be disseminated elsewhere in upcoming publications.

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