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Development and Validation of a cloud-based Digital Twin Platform of a Li-ion Batteries by means of Cell-Level Modelling

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Summary

The correct monitorisation and control of battery operating conditions such as temperature, charging profile and State of Charge operating ranges are essential to ensure safe operation and maximise battery lifetime. However, battery behaviour monitoring and modelling remains a significant technical challenge due to non-linearities and coupled phenomena governing their performance. The pursuit of new, increasingly intelligent and computationally heavy state estimation algorithms requires a significant amount of data and computational power, which at some point can be challenging to deploy in current BMS solutions, specially if hard real-time requirements are to be met on specific safety functions. To solve this problem, this paper proposes a cloud-based digital twin platform to expand computational power and data storage capacity of any given BMS solution. This work provides the description and validation of the models to be integrated into the target simulation platform and a module-level modelling approach.

Keywords: lithium battery, battery model, battery SoC (state of charge), internal resistance, optimization

1 Introduction

Maximising Li-ion battery (LIB) lifetime is a technical challenge due to the strong coupling between battery longevity and battery operating conditions such as temperature, charging profile or State of Charge (SOC) operating range [1]. Therefore, appropriate battery monitoring under a wide variety of operating conditions is essential to maximise the usability and lifetime of the batteries.

Although some research efforts are currently trying to introduce embedded sensors on Li-ion batteries [2], on this date, the internal states of a LIB are not directly measurable in situ by conventional sensors. Therefore estimations are required to quantify these X states, and the most promising are model based ones. SoC and State of Health (SoH) are some of the typical key X states (SoX) that are tracked in the Battery Management System (BMS). The monitoring of SoX allows a correct and safe operation of the battery. In addition, they provide essential information about the energy and power available. This enables advanced control strategies, advanced fault or safety condition diagnosis, thermal management or optimal control of battery performance. Accurate and robust estimation algorithms are often based on historical data, requiring greater computational power and memory that conventional industrial BMS solutions lack [3]. To overcome these challenges, the required performance of the BMS can be complemented by means of cloud computing and IoT-based technology.

With batteries becoming increasingly connected thanks to the use of Internet of Things (IoT) technologies, there is the possibility of collecting real operation data once the batteries are deployed. In this context, Digital Twins (DT) [4] are created as digital replicas of the battery with close interaction with 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) that can complement the in-field counterpart. This enables the application of key communication and networking technologies such as virtualisation, real-time monitoring and paves the way towards improved asset management and subsequently extend the battery lifetime.

With the final purpose of developing a battery DT, this work begins introducing the selected cell and the electric and thermal models developed for the design of the cloud-based simulation platform (Section 2). Continuing with the preliminary validation results of both models (Section 3). The hardware required for the validation of the developed models is then presented, along with the initial approach for the extrapolation of the models to the module level and the implementation plan of the target DTFP in the cloud (Section 4) and finally the main conclusions and future work are highlighted.

2 Developed Digital Twin Simulation Platform

In this section, the selected cell is presented together with the electrical and thermal models developed in this work. In addition, the development that followed for the proper integration of both models for the final DTSP is explained.

2.1 Selected Cell Reference

In this study, Lithium Werks 26650 cells (Figure 1) were used. Their main characteristics are summarised in Table 1.

Table 1: Lithium Werks 26650 cell characteristics.

Nominal Ratings	
Voltage	3.3 V
Capacity	2.5 Ah
Internal resistance	6 mΩ
Temperature range	-30 – 55 ºC

Figure 1: Lithium Werks 26650 cell.

Concerning issues of performance and lifetime prediction of LIBs, models of different nature are often used [5], [6]. 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.

The DTSP consists of a set of models and estimators that describe the instantaneous state of the battery. Below, the developed electrical and thermal model will be described. In order to parameterise these models, the cell had to be tested under different operating conditions.

2.2 Electric Model

Batteries are often modelled to describe the voltage response of the cells according to the different physical phenomena [1]. Equivalent circuit models (ECMs) are one of the most common methods for electrical modelling of batteries. ECMs use electrical elements such as resistors and capacitors, as well as an open circuit voltage (OCV) versus SoC profiles to reproduce the voltage response of a battery. ECMs require detailed parameter identification to represent the non-linear nature of the battery cells. They are lighter than electrochemical models and, depending on the specific battery chemistry and targeted modelling accuracy, a different number of RC pairs can be used. In this work, an ECM with two RC pairs was chosen, which also considered the hysteresis effect. This exact definition of ECM has been chosen due to its trade-off between accuracy, complexity and computational cost. Figure 2 describes the ECM to be implemented in the DTSP.

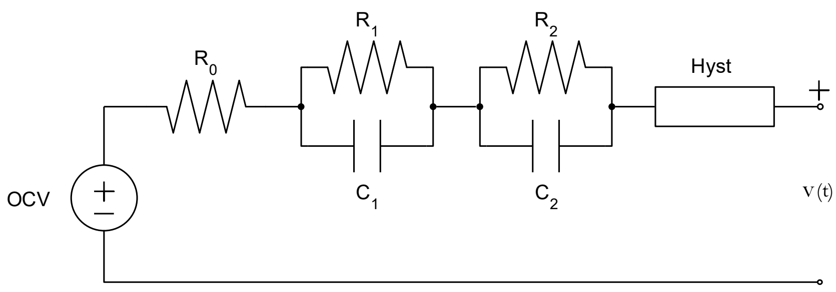

Figure 2: Digital Twin Electric Equivalent Circuit Model

The different parameters of the model are influenced by the temperature and SoC of the LIB. These parameters are obtained by different laboratory tests such as the Hybrid Pulse Power Test (HPPT) or the OCV vs SoC test. Those are then introduced in a look-up table and the model updates the value of the parameters at each time step. The states of diffusion voltage, the hysteresis voltage and the internal resistance of the cell are calculated following the same procedure as presented in [7].

The instantaneous hysteresis component changes with the sign of the input current. This hysteresis voltage is modelled by $s(k)$:

$$s(k) = \begin{cases} sgn(i(k)), & |i(k)| > 0 \\ s(k-1), & otherwise \end{cases} \quad (1)$$

M is the value of the maximum positive and negative value of hysteresis at any SoC. On the other hand, M_0 is the instantaneous hysteresis. Therefore, full hysteresis voltage will be defined as $(M_0 s(k) + Mh(k))$. The output equation of the model considers all the phenomena described above. The equation is defined in (4).

$$v(k) = OCV(k) + M_0 s(k) + Mh(k) - R_1 i_{R_1}(k) - R_2 i_{R_2}(k) - R_0 i(k) \quad (2)$$

In the batteries, states are estimated indirectly from measurement data by the BMS. The BMS must be able to choose the model parameters at each time step such as cell capacities or resistances and the different cell states such as state of charge or diffusion voltages. Estimation of SoC is complex because it is time-dependent, highly non-linear depending on battery chemistry and variable with temperature. Traditional methods for estimating SoC include the voltage-based method (open-circuit voltage (OCV)) [8] and the current-based method (coulomb counting) [9] . These types of methods for SoC estimation are simpler to implement, however, they have their limitations. The OCV method ignores the effects of impedance, diffusion and hysteresis voltage. On the other hand, the Coulomb Counting method is an open-loop type of estimation with a cumulative error.

Therefore, more advanced methods are preferred to this type of estimation techniques, such as Kalman filters, for example. In this work, a Sigma Point Kalman Filter (SPKF) has been added to the ECM model. This algorithm estimates the SoC value based on the measured voltage, current and previously estimated SoC (by means of the ECM). It is based on the sequential probabilistic inference, and results in a six steps algorithm, that can be grouped into prediction and correction phases (each one composed of three of the six steps). This algorithm produce a state estimate together with their confidence boundaries for each measurement interval. More detailed information can be found in [10], [11].

2.3 Thermal Model

Thermal models are used to describe the thermal gradient of LIBs. They can be used to estimate the temperature at different points in the cell without additional temperature sensors that increase the cost of the energy storage system. The chosen and developed thermal lumped model is shown in Figure 3.

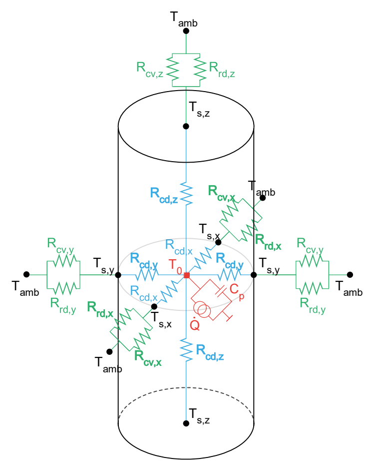

Figure 3: Digital Twin Thermal Lumped Model.

In a first step, this model calculates the heat generated by each cell $(\dot{Q}_{gen})$ and the accumulated heat $(\dot{Q}_{accu})$. In addition, the heat transferred to the cell surface by conduction $(\dot{Q}_{cd,i})$ is calculated in all three dimensions. This heat transferred to each cell surface is dissipated by convection $(\dot{Q}_{cv,i})$ and radiation $(\dot{Q}_{rd,i})$. This convection evacuated heat power is calculated using the resistance corresponding to each of the cell dimensions (radial and axial in this case). The thermodynamic energy balance of lithium-ion batteries was discussed in detail by Bernardi et al. [12]. However, not all processes were considered in this work, only heat generation, heat storage capacity, heat transfer and finally heat dissipation.

In Figure 3, the capacity C_p symbolises the thermal inertia of the cell. The different thermal resistances represent the thermal diffusion in different directions from the cell core to the different surfaces and along them. In the scenario of this work, convection occurs naturally (no cooling system is used), so it is necessary to consider the diffusion heat by radiation. To calculate this energy balance, the basic thermodynamic equations described in [14] are used.

The generation of heat ($\dot{Q}_{gen}$) is given by the result of the transfer of charges creating irreversible thermal energy loses, as well as by the reversible electro-chemical reactions in the cell. A simplified form of the equation proposed by Bernardi et al. can be used as an expression of the heat source in the lithium-ion cell adopted in this work, as shown in the following equation:

$$\dot{Q}_{gen} = I(V - U^{avg}) + IT\frac{dU^{avg}}{dT} = I^2 \cdot R_0 + I \cdot T \cdot EHC \tag{3}$$

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 (℃) and (dU^{avg}/dT) is the Entropic Heat Coefficient (EHC) in $(Volts/℃)$ defined by the variation of the equilibrium potential with temperature.

Irreversible heat is defined as the heat which behaves as an exothermic process regardless of whether the cell is charging or discharging. On the other hand, the reversible heat is the responsible of the exothermic or endothermic performance of the cell. The EHC defines the amount of heat generated or absorbed for each SoC point in the charging or discharging processes. With positive EHC values, a cell will generate heat during charging (positive current value) while it will absorb heat during discharging (negative current value) [13]. The opposite happens with negative EHC values. EHC changes are subject to each specific cell and must be studied for each case.

The equations describing each of the thermal phenomena, describing the overall thermal balance, are described as:

$$\dot{Q}_{\mathrm{accu}} = \dot{Q}_{gen} - \dot{Q}_{cond} \tag{4}$$

$$\dot{Q}_{cond,\mathrm{i}} = \dot{Q}_{conv,\mathrm{i}} + \dot{Q}_{rad,\mathrm{i}} \tag{5}$$

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

2.4 Integration of Cell Models

The models previously presented are integrated to develop a DTSP based on cloud computing. This platform is designed 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. After analysing the inputs, outputs and parameters required by each of these models, it was studied which characteristics are shared and how the basic properties of each model influence the other. As shown in Figure 4, both models require a current profile as input data and also need the temperature and the SoC from the previous step. In terms of parameters, they share a common internal resistance parameter of the cell.

In Figure 4, a simulation platform for this cell is proposed for a complete electrical and thermal monitoring. Both models are updated to obtain more accurate and reliable estimates and predictions. The parameters of each model must be chosen at all times based on the SoC and the actual temperature of the cells. This may lead, for example, to a miscalculation of the SoC estimation that could lead to a false cell heat generation and consequently, a wrong cell temperature estimation. In addition, the thermal and electrical dynamics of the cells are not equal (the electric dynamics are faster than the thermal ones) so the execution times of each of the models must be also optimised.

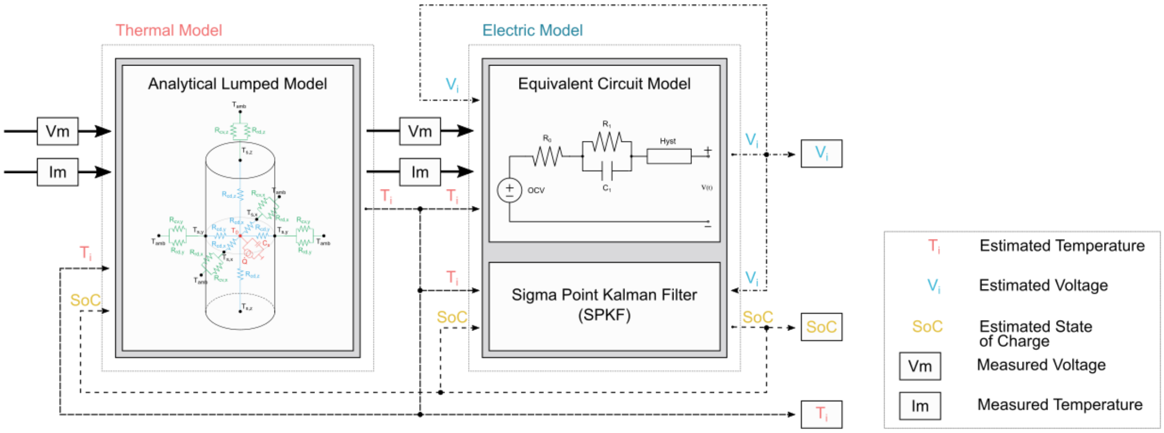

Figure 4: Digital Twin Simulation Platform.

3 Preliminary Validation Results

The DTSP validation will be done both at the cell level and battery module level. However, this paper mainly focuses on the former validation stage. For that purpose, different electric and thermal characterisation tests at Beginning of Life (BoL) were carried out.

For the electrical model validation, a HPPC test was performed in which different C-rate pulses were applied to the cells at different points of the SoC, both in charge and discharge. On the other hand, the thermal model validation was performed against a cell capacity test where the measured temperatures are compared with the thermal model estimation.

3.1 Electric Model Validation Results

To examine and compare the performance of the proposed algorithms, a discrete-time state-space model applied to the battery cells was first defined. Tests were performed in the laboratory to adjust the parameters of the cell model, and then tests were performed on another cell to see how these models fit the cell performance. For the tests, a climatic chamber was used for the experiments requiring a constant temperature and a programmable Industrial Battery Tester (IBT).

The cell test carried out were a sequence of 4 charge and discharge pulses (of 2.5 A and 1.25 A) spread over the SOC range of 90-10%, all at ambient temperature of 25°C. Figure 5(a) represents the SoC as a function of time while charging and discharging, the measured voltages and voltage estimation in Figure 5(b) and finally in Figure 5(c) the absolute error of the model in mV.

The actual voltage value (blue line) was compared with the predicted voltage value (orange line) for the tested data. The model fit has been evaluated by comparing the estimation error (equal to the cell voltage minus the model predicted voltage) and a very close agreement is observed, especially during the dynamic part of the test. The mean absolute error of the model prediction is 0.0228 mV and the maximum error of 0.7291 mV, only taking place at very low SoC levels in which the performance of the voltage response of the cell significantly varies from its behaviour at greater SoC values.

In the specific case of this cell, the cell's voltage or response is very significant at both edges (0% and 100% SoC). There are two main reasons for these: i) the size of the cell and ii) the distinctive OCV curve of the cell. Due to this variation, a small error in the SoC estimation is produced at low SoCs, e.g. the model arrives to 1% SoC instead of 0%. These errors have led to a deviation in the estimates in the charging part of the test. Especially at the high SoC part, where the model predicts that the cell reaches its 100% SoC earlier than it should.

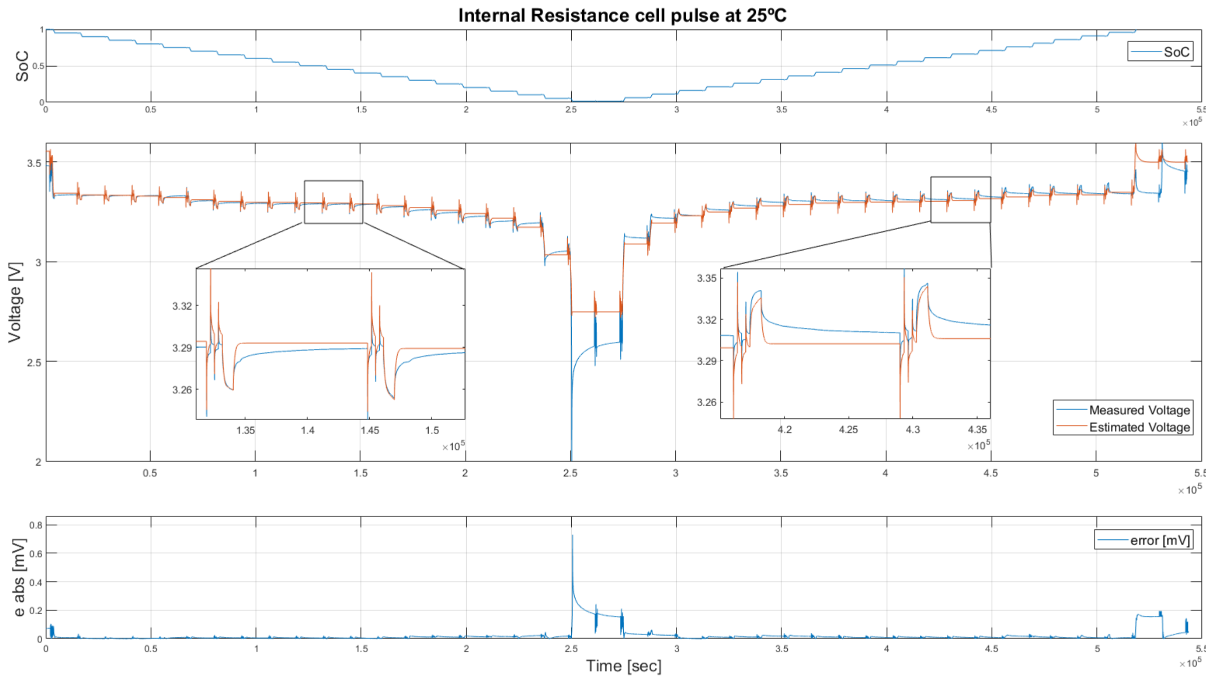

Figure 5: Results of ECM at 25 ºC.

On the other hand, the test has been repeated with an identical current profile at an ambient temperature of 45ºC. Figure 6 shows the results obtained by the electrical model under the new conditions.

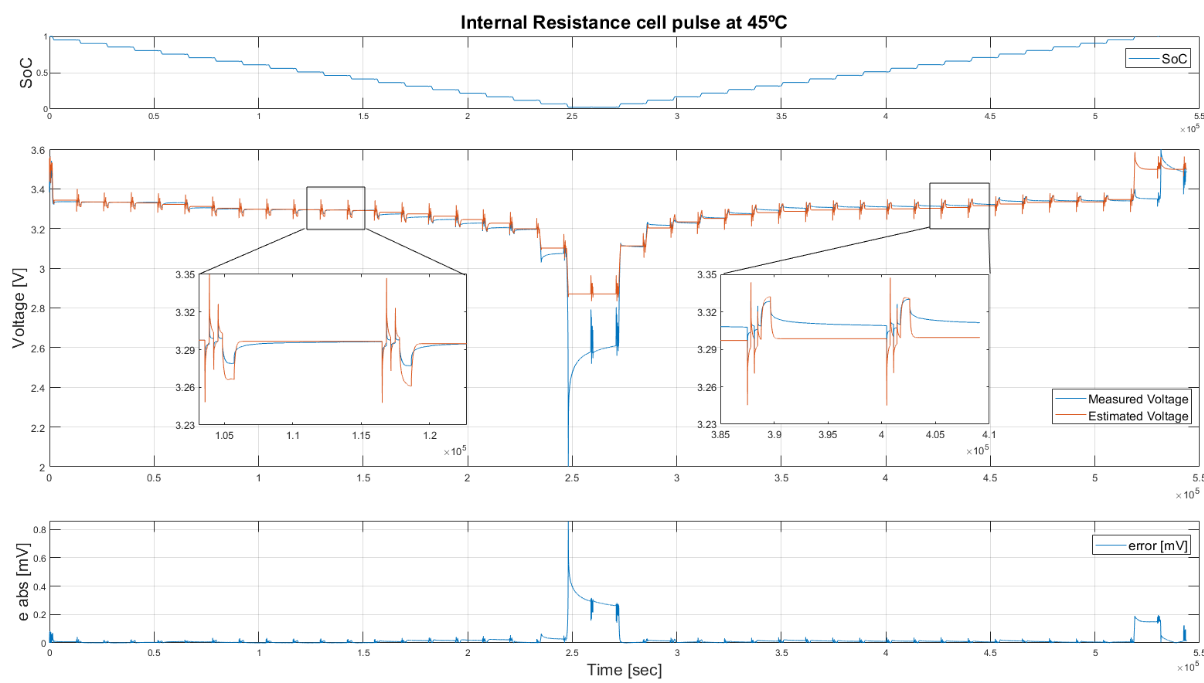

Figure 6: Results of ECM at 45 ºC.

The model has mostly predicted the correct voltage value with a mean absolute error of 0.0275 mV and the maximum error of 0.8574 mV. These results prove the validity of the electrical model, which is well suited to subsequent simulation needs at battery module level. Further validation results will be reported in upcoming publications.

3.2 Thermal Model Validation Results

In this part, the identified thermal behaviour of the selected cell was further analysed by means of loads at different C-rates. In this way, the expected performance and the thermal response measured during the testing of the cell could be verified. 1C load of two complete cycles of the cell was performed in a thermal chamber at a constant ambient temperature. The thermal chamber used has an accuracy of ±0.3 ºC to maintain the desired ambient temperature. The temperature mapping of the cell temperature was performed using T-type thermocouples for each cell surface with an accuracy of ±1.5 ºC and the IBT was used to load the cells. The same test was then repeated, in this case at 4C.

The thermal model calculates an energy balance at each time step to estimate and optimise the temperatures of every surface of the cell. The energy balance is performed using the Newton Raphson optimisation method. Figure 7(a) represents the SoC as a function of the cell, the measured temperatures and the temperature estimation by the model in Figure 7(b) and finally in Figure 7(c) the absolute error of the model in ºC of the two tests.

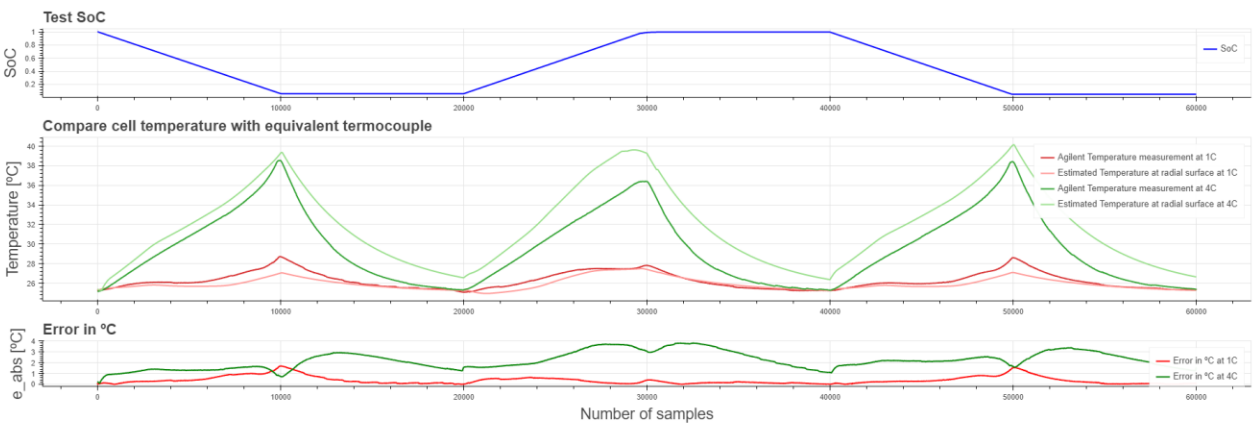

Figure 7: Results of Lumped Model for 1C current profile.

The model has an average error of 0.3609 ºC and the maximum error of 1.7093 ºC. This same test has been repeated in this case at 4C currents of the cell. The model was not parametrised for such high currents, however it showed an acceptable accuracy with an average error of 2.3405 ºC and the maximum error of 3.8244 ºC. Thus, it was concluded that the model is able to predict the temperature at different operating C-rates with a sufficient accuracy.

4 Implementation of the DTSP in the Cloud

To develop module-level battery models which consider each of the cells separately, this section will describe in detail the proposed module-level modelling approach. Most of the electrical and thermal battery modelling works in the literature are designed and validated at the cell level. However, the actual performance of a DTSP depends on its ability to model LIB performance at the module level. To implement this methodology, the proposed hardware is presented in Figure 8.

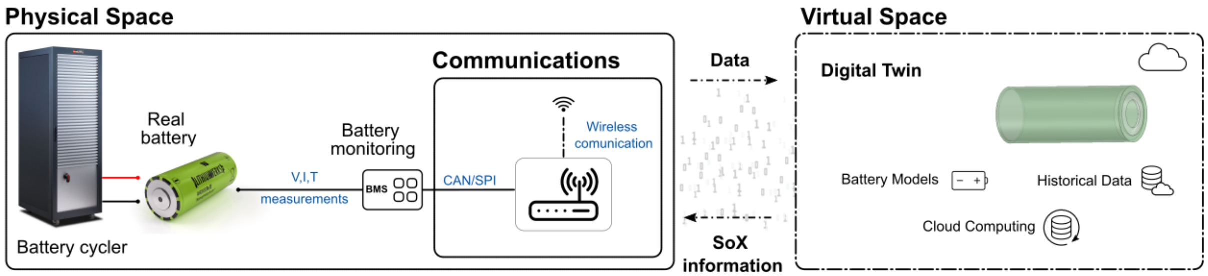

Figure 8: Schematic diagram of the proposed DTSP validation platform.

A battery module is composed of a series of cells connected in series or parallel. However, all these cells rarely operate in perfect balance when it is operating, and this affects the final useful energy of the battery. Therefore, it is necessary to estimate the SoX of each cell and then estimate the equivalent response of all the cells. To this end, this work is ongoing on the extrapolation from cell-level models to full module-level models.

In this line, it is proposed to develop the thermal model presented in this work and extrapolate it to make its estimations at the module level. By implementing at the module level, the heat transferred between all the cells is considered. 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 the core temperature of each cell are obtained. These are used to decide the equivalent temperature of each cell. The thermal model at module level uses the updated voltage and SoC information (information estimated by the electrical model). In turn, temperature is known to influence the electrical behaviour of the cell, so the temperatures estimated and updated by the thermal model will be used as input for the electrical models at the cell level. The electrical model is implemented for each cell and co-simulated. The results are extrapolated to the module level considering some previously defined criteria for the estimation of the Equivalent Module Voltage (EMV) and this successively to estimate the equivalent SoC of the whole module.

The DTSP will provide a clearer representation of the temperature distribution over a large number of points within the module, which is usually not affordable as LIB modules typically have a small number of temperature sensors. In addition, this platform allows for a more accurate estimation of the SoC of each cell in the module. This, together with the temperature distribution, can lead to more accurate SoH and RUL estimates. Moreover, the simulation of the whole module performance can contribute to identify unexpected behaviours on the real battery system – e.g. an excessive temperature measurements compared to the simulation results (at certain operating conditions) – thus potentially contributing to prevent hazardous safety events. However, running the thermal model at the module level (the calculation of the energy balance multiplied by the number of cells) together with electrical co-simulations at the cell level requires considerable computing power that the battery BMS may not be able to provide.

To overcome these challenges, the required performance of the BMS can be extended by means of cloud computing technologies. With this computational capacity, continuous monitoring with different state estimation algorithms is possible.

Thus, Cloud Computing technology will be used for the implementation of the designed DT which is expected to reach close to real-time operation performance. To develop the Cloud, it was decided to use the Amazon Web Services as cloud infrastructure provider. The developed architecture is presented in Figure 9.

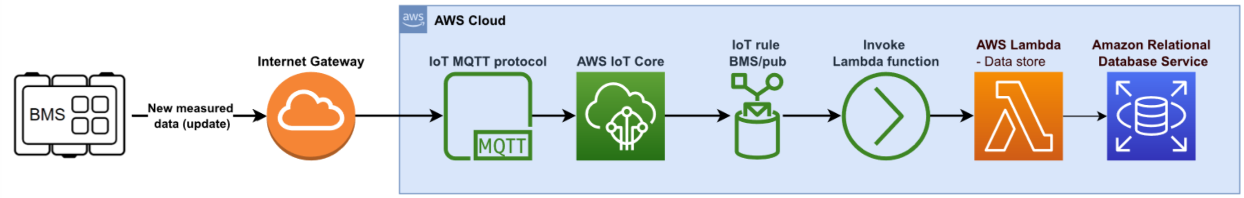

Figure 9: Schematic architecture of the DTSP Cloud's acquisition of new measurements.

The data obtained by the BMS will be sent by means of a simple gateway to the Cloud. Message Queuing Telemetry Transport (MQTT) communication protocol and the AWS IoT service will be used to make this connection. Each time AWS IoT receives a new input, it will trigger a Lambda function automatically. This data will then be stored in a relational database and finally the DT algorithms will be executed allowing the monitoring of the LIBs in real time as shown in Figure 10.

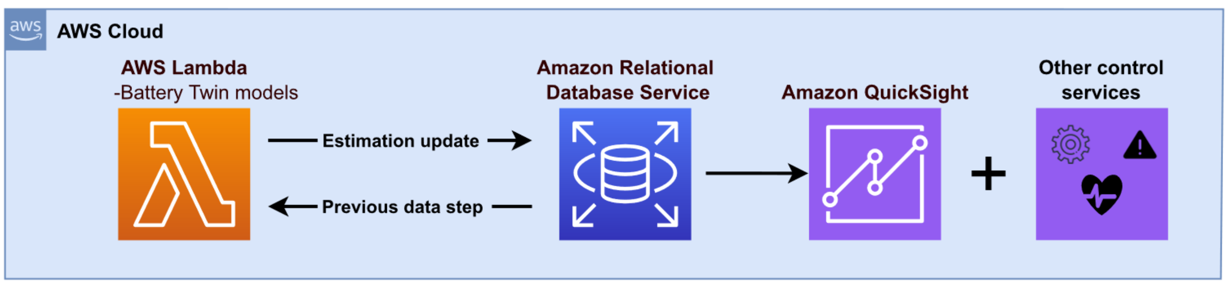

Figure 10: DTSP Cloud schematic architecture

As previously mentioned, the models need data from previous estimates, so the Lambda function will call the database and update with the new estimates performed. All SoX estimates will be stored in historical data and will allow the monitoring of LIBs in real time. Finally, a visualisation service (Amazon QuickSight) and other monitoring services will be used. Additional services such as predictive maintenance or a series of alarms and warnings for both the manufacturer and the end-user are under consideration.

5 Conclusions

This paper describes the initial stage of the development of a DTSP for LIB, mainly meant to extend computation and computation power capabilities of current BMS solutions.

Cell-level electric and thermal battery models were developed. Both electric and thermal LIB models were validated under experimental data obtained in laboratory tests in a DTSP framework at the cell level. Results obtained highlight the tight coupling among models and provide a baseline modelling framework for subsequent development stages, comprising a thorough module-level modelling approach.

Additionally, the DTSP validation platform currently being developed was presented, besides the constructed cloud architecture where the developed cell-level (and subsequently module-level) models will be deployed. The DTSP framework here described takes advantage of extended cloud computation capabilities to extrapolate individual battery models to a battery module level, ultimately allowing extended monitoring capabilities.

Results presented in this paper will be further developed and reported on upcoming publications in which the advantages of module-level approaches will be contrasted to simpler cell-level approaches most widely used to this date.

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