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FASTEST

Fast-track hybrid testing platform for the development of battery systems

Deliverable D2.1: Use case specific battery testing boundary conditions and DOE methods

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Project Abstract

Current methods to evaluate Li-ion batteries safety, performance, reliability and lifetime represent a remarkable resource consumption for the overall battery R&D process. The time or number of tests required, the expensive equipment and a generalised trial-error approach are determining factors, together with a lack of understanding of the complex multiscale and multi-physics phenomena in the battery system. Besides, testing facilities are operated locally, meaning that data management is handled directly in the facility, and that experimentation is done on one test bench.

The FASTEST project aims to develop and validate a fast-track testing platform able to deliver a strategy based on Design of Experiments (DOE) and robust testing results, combining multi-scale and multi-physics virtual and physical testing. This will enable an accelerated battery system R&D and more reliable, safer and long-lasting battery system designs. The project's prototype of a fast-track hybrid testing platform aims for a new holistic and interconnected approach. From a global test facility perspective, additional services like smart DoE algorithms, virtualised benches, and DT data are incorporated into the daily facility operation to reach a new level of efficiency.

During the project, FASTEST consortium aims to develop up to TRL 6 the platform and its components: the optimal DOE strategies according to three different use cases (automotive, stationary, and off-road); two different cell chemistries, 3b and 4 solid-state (oxide polymer electrolyte); the development of a complete set of physic-based and datadriven models able to substitute physical characterisation experiments; and the overarching Digital Twin architecture managing the information flows, and the TRL6 proven and integrated prototype of the hybrid testing platform.

LIST OF ABBREVIATIONS, ACRONYMS AND DEFINITIONS

Acronym	Name
BMS	Battery Management System
CCD	Central Composite Design
DOE	Design of Experiments
EOL	End of Life
FIM	Fisher Information Matrix
HPPC	Hybrid Pulse Power Characterization
OCV	Open Circuit Voltage
PDE	Partial Differential Equation
PI-DeepONet	Physics-Informed Deep Operator Network
PINN	Physics-Informed Neural Network
RSM	Response Surface Methodology
SOC	State of Charge
SPM	Single Particle Model
WLTP	Worldwide Harmonized Light Vehicles Test Procedure

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1. EXECUTIVE SUMMARY

Deliverable D2.1 is a crucial document within the FASTEST project that is describing the boundary conditions, success criteria and objectives of the three use cases "automotive", "energy storage systems" and "off-road mobile" and identifies and describes their distinct nature when it comes to the experimental design of battery tests.

Furthermore, D2.1 aims at providing an extensive overview over the broad scientific landscape that is labeled by the design of experiments (DOE) in order to ultimately identify those methodologies that are most promising for contributing towards the different workflows within the FASTEST platform.

The evaluation of both use-case specific boundary conditions and objectives as well as existing DOE methodologies highlights that only the combination of use-case-specific knowledge with novel DOE methodologies can provide a toolbox that can ultimately help in reaching the ambitious goals that have been proposed for the FASTEST project.

In conclusion, Deliverable D2.1 provides an extensive overview over both the considered use-cases as well as state-of-the-art DOE methodologies, effectively paving the way for a fruitful combination of the two elements within novel and intelligent DOE methodologies which are specifically tailored to respect the distinct nature and boundary conditions for battery testing in each use case. All of this is done with a clear goal of minimizing testing time and costs throughout the whole development process of battery systems.

2. OBJECTIVES

Some of the key objectives of the FASTEST project include a reduction of operating time and costs via a hybrid testing platform that utilizes optimized DOE methodologies. This goal is closely related to another objective that aims at a high overall ratio of fully virtualized test. Both of these aspects can only be achieved by virtual models that are properly and trustfully parametrized, which emphasizes the need for state-of-the-art models but also a DOE methodology that allows state of the art parametrization of such models while being specifically tailored towards the different use cases covered within the FASTEST project.

In order to push towards those ambitious goals within FASTEST, D2.1 builds upon previous work from WP1, where different use cases as well as their boundary conditions, regulations and digitalization potentials have been summarized and evaluated. In the context of WP2, D2.1 serves as a first step towards the development of battery testing procedures based on intelligent DOE by screening and evaluating previous work in the broad landscape of DOE methodologies. This is done both for general purposes but also in specific applications for testing and the development of LIBs in order to identify application areas and objectives that are in line with the aforementioned objectives of the FASTEST project. In close collaboration with other work packages such as WP3, the most promising methodologies and DOE aspects have been identified and further evaluated with respect to the roadmap of the FASTEST project.

Consequently, the Deliverable concludes with a proposed workflow and some preliminary results that may serve as a baseline for the next stages of the project where the use-case specific requirements and boundary conditions need to be fully integrated into an intelligent DOE-based battery testing procedure that is specifically tailored and optimized for each considered use case.

3. INTRODUCTION

In the development and evaluation of battery systems, establishing a robust methodological framework is crucial. This framework should not only understand basic behaviors of these systems but also predict their performance under specific use conditions. The FASTEST project's approach to creating a hybrid testing platform aims to achieve this goal by integrating physical tests and virtual simulations to optimize the reliability and economy of the battery development process.

This document, Deliverable D2.1, details the specific testing conditions for batteries and the Design of Experiments (DOE) methods that have been tailored for three differentiated use cases: automotive, stationary energy storage, and off-road mobile devices. Through a combination of physical tests and high-fidelity virtual models, this integrated approach seeks to overcome the traditional challenges associated with isolated experimentation, such as high time and resource demands, and difficulty in simulating varied operational conditions.

The methodological framework proposed in this document is based on interdisciplinary collaboration and innovative use of DOE techniques to assess and enhance the design and performance of battery systems. The implementation of these methodologies in a hybrid testing environment is discussed, highlighting the synergy between detailed simulations and rigorous physical testing. This approach not only increases the accuracy of test results but also provides a solid foundation for decision-making in battery development, ensuring that systems not only meet current requirements but are also ahead of future needs.

Additionally, the challenges encountered in integrating these methodologies are addressed, and strategies adopted to mitigate them are outlined, ensuring that the FASTEST project can provide practical and effective recommendations for the battery system industry. With this comprehensive approach, the project seeks not only to improve current testing methods but also to establish new standards in battery evaluation for a variety of applications.

4. BATTERY TESTING BOUNDARY CONDITIONS

The first part of the work description within this Deliverable is focused on the use case specific battery testing boundary conditions. Three different use cases were selected in order to validate and apply the innovative methodologies developed within FASTEST in real application scenarios. In previous work within the FASTEST project, testing procedures, regulations and standards were identified for the different use-case and evaluated with respect to their virtualization potential within the consortium of FASTEST. In order to differentiate between tests that are applicable to the considered battery cells regardless of their final application scenario and such tests that are indeed use-case specific and require tailored DOE approaches, this section is split into two parts. First, a general overview on testing procedures applicable to any use case of our considered battery cells is presented.

4.1 General Testing Boundary Conditions

Standardized test protocols have been developed to establish general boundary conditions for Type 3b battery cells. The purpose of these conditions is to ensure that all battery cells undergo a uniform set of tests that assess their performance and longevity under a range of operating conditions reflective of real-world scenarios. This promotes comparability and reproducibility of results between different battery systems and helps identify areas for continuous improvement in battery design and management. These tests are conducted at temperatures of 15°C, 25°C, and 45°C to simulate various operating environments.

Based on the potential tests studied in WP1, a series of tests have been selected for both the creation of necessary models in WP3 and WP4, as well as for potential physical tests that will be performed on test benches once the hybrid platform is finalized and all its components are interconnected. The tests are divided into two sections, performance test and safety test. The selected tests are outlined as follows.

It should be noted for the following sections, that all the tests mentioned are developed in depth in WP3, this deliverable does not go in depth into each of the tests and their procedures.

Furthermore, although the boundary conditions for the cells of the FASTEST project may be defined, the ultimate goal of the project is the creation of a platform that can work for different types of cells and modules, therefore these boundary conditions will always depend on the specifications of the product to be tested.

4.1.1 Performance Tests:

Preconditioning Test:

This process involves charging battery cells to their maximum specified voltage and discharging them to a predetermined state of charge (SOC). The cells undergo a stabilization period at specific SOCs to allow for thermal and electrical equilibrium, conducted at 15°C.

<u>Boundary Conditions:</u>

Voltage Levels: Cells charged to their maximum specified voltage.

Discharge Level: Cells discharged to a specified percentage of SOC.

Current Rates: Constant current adapted to the cell's capacity and discharge characteristics.

Temperature: Tests conducted at 15°C, 25°C, and 45°C temperatures to evaluate thermal effects.

Stabilization Period: A rest phase at a specified SOC to allow for thermal and electrical stabilization.

Capacity Test:

Cells are charged to their maximum voltage and then discharged to the manufacturer-specified cut-off voltage. The entire test is performed under a stable ambient temperature, at 15°C, 25°C, and 45°C, with a constant current rate that is adapted to the cell’s specifications.

<u>Boundary Conditions:</u>

Voltage Levels: Charging up to the cell's maximum voltage and discharging down to the manufacturer-specified cut-off voltage.

Current Rates: Constant current rate, adapted to the cell’s specifications.

Temperature: Test conducted at a stable temperature.

OCV Charge Test:

The open circuit voltage (OCV) profile of the battery is assessed by charging from a low specified voltage up to the cell's maximum voltage. The cell rests at various SOC levels during the test to measure voltage stabilization, conducted at 15°C, 25°C, and 45°C.

<u>Boundary Conditions:</u>

Voltage Range: From a low specified voltage up to the cell's maximum voltage.

Rest Periods: Resting the cell at various SOC levels to measure voltage stabilization.

Temperature: Conducted at standardized temperatures to assess thermal effects.

OCV Discharge Test:

This test measures the voltage profile as the battery discharges from its maximum voltage down to a specified lower voltage limit. Rest periods are included at various SOC points to observe voltage changes, carried out at standardized temperatures of 15°C, 25°C, and 45°C.

Boundary Conditions:

Voltage Range: From the cell's maximum voltage down to a specified lower voltage limit.

Rest Periods: Cell rested at various SOC points to observe voltage changes.

Temperature: Test carried out at standardized temperatures.

HPPC Test:

This test evaluates the battery's power capability, especially its ability to handle brief high-current loads and recover. It includes short high-current pulses alternated with rest or low-current periods, and voltage drops and recovery are critically monitored. The HPPC test is performed at 15°C, 25°C, and 45°C.

Boundary Conditions:

Pulse Current: Short high-current pulses alternated with rest or low-current periods.

Voltage Monitoring: Critical to record voltage drops and recovery after pulses.

Temperature: Conducted at various standardized temperatures.

Thermal Test:

The thermal test involves taking measurements at various points within the battery cell simultaneously, specifically targeting six different points to understand its thermal behavior comprehensively. This method assesses the battery's performance under various environmental conditions. The test controls the heating and cooling rate to prevent thermal shock while monitoring key performance indicators such as capacity, voltage, and internal resistance at each measurement point. These generic boundary conditions provide the flexibility to adapt the test to specific cell specifications, ensuring precise and relevant data collection and analysis for various battery types.

Generic Boundary Conditions:

Temperature Range: Tests conducted through a defined range of temperatures.

Heating/Cooling Rate: Controlled to avoid thermal shock.

Measurement: Monitoring performance in terms of capacity, voltage, and internal resistance at each temperature.

These generic boundary conditions allow flexibility and can be tailored to specific cell specifications when conducting tests, ensuring accurate and relevant data collection and analysis for a variety of battery types.

4.1.2 Safety Tests:

Safety tests are designed to evaluate the robustness and safety features of battery cells under extreme or faulty conditions. These tests are crucial for ensuring the reliability and safety of batteries in various applications. The tests include scenarios such as overcharge, forced discharge, internal and external short circuits, continuous charging, extreme heat exposure, thermal cycling, cooling system failures, moisture resistance, internal fires, high-rate charging, and working voltage measurements.

Cell level

Overcharge Test:

This test involves charging a battery beyond its maximum rated voltage to assess the safety mechanisms and robustness under conditions that might occur during abnormal charging scenarios. The objective is to ensure that the battery can safely handle excessive voltages without catastrophic failure, such as thermal runaway or cell rupture.

Forced Discharge Test:

The forced discharge test subjects the battery to discharging at rates higher than the manufacturer's specifications to evaluate the battery's ability to safely dissipate energy. The goal is to confirm that the battery maintains structural and chemical integrity when subjected to stress beyond its normal operational capacity.

Internal Short Circuit Test:

This test simulates an internal short circuit within the battery to examine how well the battery can contain and control the heat and potential ignition that might result from such a fault. It assesses the effectiveness of the battery's internal design and safety features in preventing a fire or explosion.

External Short Circuit Test:

In this test, an external short circuit is deliberately created to observe the battery's response. The aim is to test the external safety measures and circuit protection to ensure they react appropriately to prevent damage and ensure user safety.

Continuous Charge Test:

This test involves continuously charging the battery without a typical cut-off to see how the battery handles overcharging scenarios. It evaluates the effectiveness of the battery management system in preventing overcharging and maintaining safety.

Working Voltage Measurement Test:

This test measures the operating voltage range of the battery under normal use conditions to establish baseline performance metrics. The goal is to ensure the battery operates safely and effectively within the designated voltage parameters.

Extreme Heat Test:

The extreme heat test exposes the battery to abnormally high temperatures to evaluate its thermal management systems and material integrity under heat stress. It's crucial for verifying that the battery can operate safely in hot climates or during intense operational heat.

Thermal Cycling Test:

This test involves repeatedly cycling the battery between two extreme temperatures to assess how temperature fluctuations affect the battery's performance and lifespan. The objective is to ensure the battery can withstand varied thermal environments without degradation.

Module level

Failure of Cooling System Test:

This test assesses the battery's behavior in the event of a cooling system failure. It helps in understanding the battery's intrinsic safety measures to dissipate heat and prevent thermal runaway when external cooling fails.

Moisture Resistance Test:

The moisture resistance test exposes the battery to high humidity or direct contact with water to evaluate its seals and coatings. The goal is to ensure the battery remains safe and functional even when exposed to moisture.

Internal Fire Test:

This test investigates the battery’s ability to contain and manage a fire within its cells or modules. It is crucial for assessing the risk mitigation strategies embedded within the battery design to protect against internal fires.

High-Rate Charge Test:

This test subjects the battery to charging at a higher current rate than usual to determine how quickly the battery can be charged safely. It assesses the rapid charging capabilities and the thermal and voltage responses of the battery under such conditions.

Working Voltage Measurement Test:

Similar to the earlier test, this involves measuring the voltage output during operational conditions to verify that the battery operates within safe and efficient voltage ranges under different loads.

<u>Generic Boundary Conditions:</u>

Voltage Levels: Testing includes pushing the voltage beyond the cell’s normal operating range to simulate overcharge and extreme conditions.

Current Rates: Applying currents that exceed the usual operational levels to assess the cell's response to overcharge and high-rate charge scenarios.

Temperature: Tests are conducted at multiple temperatures to simulate different environmental conditions and assess the battery’s thermal management and response to extreme heat and thermal cycling.

Environmental Stress: Exposure to moisture and controlled environmental failures to test the battery’s resistance to humidity and its cooling capabilities under duress.

Each test is tailored to trigger specific safety mechanisms within the battery, ensuring that all potential failure modes are adequately assessed. The use of standardized temperatures helps in evaluating the cell's performance and safety under varying thermal conditions, crucial for applications across different climates.

In the following, we describe the use-case specific battery testing boundary conditions identified for the three use cases in more detail.

4.2 Use-Case Specific Boundary Conditions

In this section, we address the specific test conditions for the three use cases considered in the FASTEST project. These conditions are designed to reflect the operational environments and unique challenges associated with each application, thereby allowing for more accurate and relevant testing and evaluations.

Therefore, in addition to the standard tests described in Section 4.1, we have designed a series of aging tests specific to each of the three identified use cases: electric vehicles, stationary energy storage systems, and off-road mobile devices. These tests are intended to simulate the charging and discharging profiles that the batteries would experience in their specific applications, thus providing a more accurate assessment of their durability and behavior under prolonged usage conditions.

4.2.1 Automotive

Recognizing the importance of evaluating battery durability and performance under realistic conditions, the implementation of the Worldwide Harmonized Light Vehicles Test Procedure (WLTP) is employed as the foundation for aging tests in electric vehicles. This contemporary standard reflects daily vehicle use more accurately and incorporates a broader spectrum of operational conditions.

Aging tests under the WLTP cycle are designed with the following specific boundary conditions:

- Speed Profiles: These include low speeds in urban areas and higher speeds typical of highways, simulating a variety of driving scenarios.

- Ambient Temperature: The tests are conducted over a range of temperatures, simulating various climatic conditions a vehicle might encounter during operation.

- Use of Auxiliary Systems: The impact of systems such as air conditioning and lighting is considered, which can significantly affect the battery's energy demand.

- Charge and Discharge Cycles: The cycles implemented reflect overnight charging and rapid recharging during the day, typical of an electric vehicle user's routine.

- Test Duration: Batteries are subjected to repeated WLTP cycles until a specific percentage of degradation of the original capacity is reached, allowing for the assessment of lifespan under continuous use.

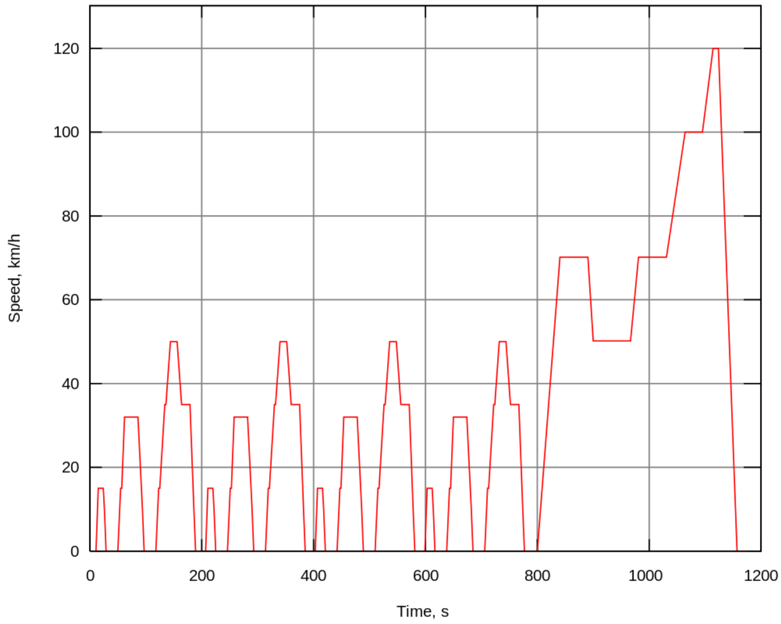

Figure 1. WLTP profile.

The End of Life (EOL) criterion is a crucial factor to consider when discussing the aging of batteries. For batteries in the context of WLTP testing is generally marked when the battery's capacity degrades to 70-80% of its original capacity. This criterion, while not specifically defined by the WLTP, is widely accepted in the electric vehicle industry. It reflects significant reductions in battery performance, notably in its ability to store and deliver energy, which directly impacts vehicle range and usability. EOL assessment involves repeated deep discharge and charge cycles to measure when the battery no longer meets these performance thresholds.

By using WLTP in aging tests for electric vehicles, it is ensured that the batteries are evaluated and optimized to perform efficiently across the full spectrum of driving conditions that end-users will experience. This approach not only enhances the relevance of the tests but also boosts consumer and manufacturer confidence in electric vehicle technology, promoting its adoption and acceptance in the global market.

The automotive use case considers a system based on 400V and 60kWh capacity with modules of 48-60 V, 100-270 A, connected in series. Its main objectives are to improve the battery systems design with respect to time and cost by utilizing the hybrid testing approach developed in FASTEST.

4.2.2 Stationary energy storage

For the stationary energy storage use case, no standardized test protocol like the WLTP for vehicles exists that specifically applies to the operational patterns of stationary storage systems. Consequently, to ensure the aging tests for this use case are conducted under realistic and scientifically rigorous conditions, a normalized current profile derived from reliable sources will be used. This approach allows for a consistent evaluation of battery performance and durability across various systems and conditions.

- Current Profile: The test utilizes a current profile that is normalized based on industry benchmarks and reliable data sources. This profile includes typical charge and discharge cycles that stationary storage systems would experience during regular operation.
- Temperature Variability: Tests are conducted under a variety of thermal conditions to simulate different environmental impacts on the storage system. Understanding how temperature influences battery efficiency and degradation over time is crucial for these systems.
- Continuous and Intermittent Cycling: Reflecting real-world usage of stationary storage, the profile includes long-duration discharges followed by full recharges, as well as intermittent, partial charge and discharge cycles to mimic demand-response scenarios.
- Test Duration: The automotive use case where a strict 70-80% capacity degradation criterion is used to determine EOL, the test duration for stationary storage systems is less stringent. Batteries are cycled until they show significant degradation, but not necessarily confined to the 70-80% range. This flexibility acknowledges the different operational stresses and longevity expectations specific to stationary applications.

By implementing normalized current profiles from reliable sources, the aging tests for stationary energy storage systems ensure consistent and replicable testing conditions that closely align with real-world demands placed on these systems. This strategy enhances the tests' relevance, providing stakeholders with confidence in the performance and longevity of these systems, ultimately supporting their broader adoption and integration into energy networks. The less stringent EOL criterion reflects the unique requirements and usage patterns of stationary storage systems, allowing for a more tailored approach to evaluating their performance and durability.

The stationary energy storage use case considers systems built from modules of 48–60V, 30-40 A and 5-10 kWh capacity, which are connected in series and parallel. As applications of such systems and therefore customer requirements may vary a lot, this use case aims for a high versatility and range of boundary conditions during battery testing and to improve the battery system design thanks to the hybrid testing approach.

4.2.3 Off-road mobile devices

Similar to the stationary energy storage use case, there is no standardized cycling protocol for off-road mobile devices. However, one of the main differences to the energy storage use case is the high scenario predictability with regularly alternating charging and discharging cycles with little dynamics and deviations. This allows to incorporate utilization data for within the aging testing of a given scenario. Within the FASTEST project, typical scenarios feature devices like Laser-Guided Vehicles (LGVs) and Automated Guided Vehicles (AGVs). The considered boundary conditions include:

- Current Profile: Normalized Current Profiles with alternating constant-current charge and discharge cycles. The working cycles remain in a narrow SOC window from 70% to 80%.
- Temperature Variability: Due to the high scenario-predictability and small considered SOC ranges, comparably small temperature variations are considered from around 25°C to 35°C.
- Test Duration: The EOL criteria are based on standard *IEC 62620:2014* and include a remaining capacity of 60% compared to the rated capacity after 500 cycles as well as an internal resistance below two times the initial resistance after 2000 cycles.

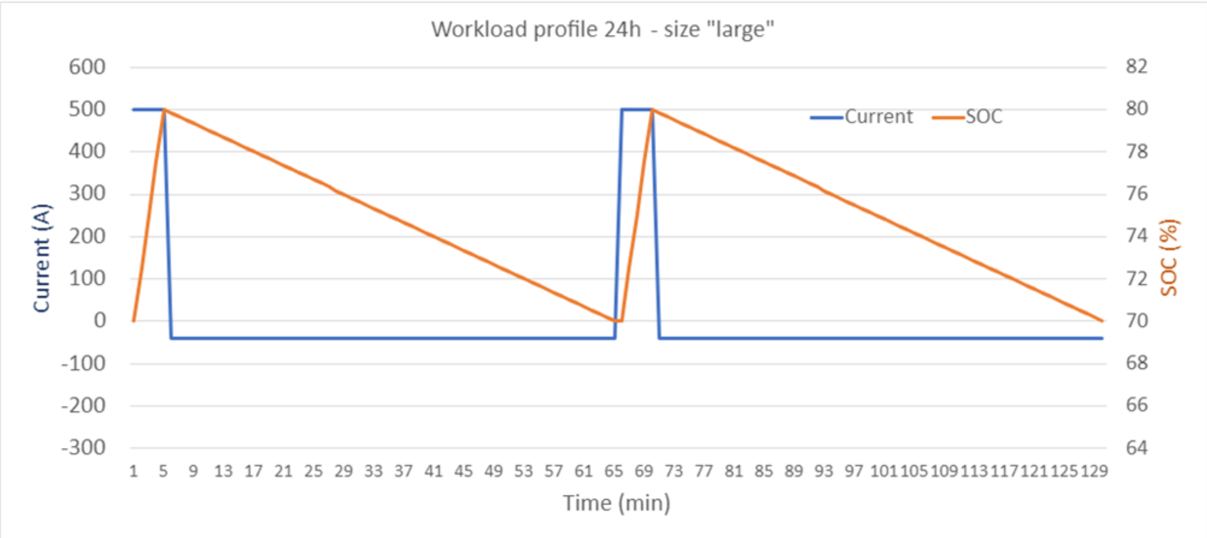

Figure 2. Exemplary Load Profile for large off-road mobile device.

This offroad/industrial use case considers systems based on 51.2V and 21.5-30.7kWh capacity with modules of 3.2-6.4V and 400-560A which are connected in series and parallel. Our main objectives are to create a customized testing protocol that leverages the insights from the battery usage dataset and optimize the battery systems testing with consider to time and cost. Figure 2 shows an exemplary current profile for an exemplary off-road mobile device.

5. DOE METHODOLOGIES

Design of Experiments (DOE) is a powerful tool in scientific research to analyze the relationship between factors (input) and responses (output) of a system. This approach is helpful to reduce time and effort of the experiments and to combine them with modelling. In the following, the general DOE methodology and some of its most important associated terms are introduced. Subsequently, the usage of DOE for different aspects related to Lithium-ion batteries (LIBs) is reviewed to provide a broad picture of different aspects and possible application scenarios of DOE. Finally, this Section concludes with an in-depth explanation of a potential DOE workflow that is tailored towards the scope of the FASTEST project.

5.1 Introduction to DOE

In general, any DOE methodology consists of a set of sequential steps which may be partially repeated based on intermediate conclusions about the problem at hand. After an initial definition of a problem statement, the relevant response variables as well as their influencing factors and levels (i.e. the considered parameter space) need to be defined. For the experimental design one may choose from a wide range of options including designs used to obtain a general understanding of the factor-response correlations, usually considering a limited set of factors and levels ("screening" or "factorial" designs). More elaborate approaches include the so-called response surface methodology (RSM) which corresponds to a contour plot in k+1 dimensions for a selected set of k factors (e.g. identified from a previous screening design). Different types of RSM designs exist, with the central composite design (CCD) being one of the most popular ones consisting of a factorial design with additional axial and centre runs, cf. e.g., [1]. Some further types and derivations of the aforementioned designs are excluded here for the sake of brevity.

Apart from classical designs, many designs exist under the general terminology of "optimal designs" which usually refers to designs that are optimal with respect to certain criteria related to information matrices and regression coefficients. In this context, the so-called Fisher-based optimal experimental designs, which are based on the Fisher-Information-Matrix (FIM), play an important role for the remainder of this Deliverable and will therefore be explained in more detail in Section 5.3.2. Table 1 provides a non-exhaustive overview over some of the aforementioned experimental designs.

After factors, responses and a specific design have been selected in the initial planning stage of the DOE workflow, experimental runs are executed, often yielding preliminary conclusions that can be re-integrated into the experimental design or the selection of factors and response for further considerations. In this sense, DOE is not necessarily a purely sequential procedure but should be viewed as an iterative process with the overall goal of fine-tuning the experimental design towards a specific objective.

Design	**Description**	**# experiments**
Screening	k factors with 2 levels each	N = 2^k
Factorial	k factors with L levels each	N = L^k
Response surface methodology	Contour plot in k+1 dimensions	N = k^2 + 2k + c (CCD)
Fisher-based optimal designs	designs that optimize the Fisher-Information-Matrix with respect to certain metrics (trace, determinant, etc.)	Non-deterministic, problem-dependent

Table 1: Overview on Experimental Designs.

Finally, another important DOE element is the statistical analysis of the experimental runs and the resulting models from which certain conclusions are to be drawn. Statistical concepts like P-value or F-value criteria can be used to back up conclusions with a solid theoretical basis by quantifying the statistical significance of the observed outcomes and conclusions.

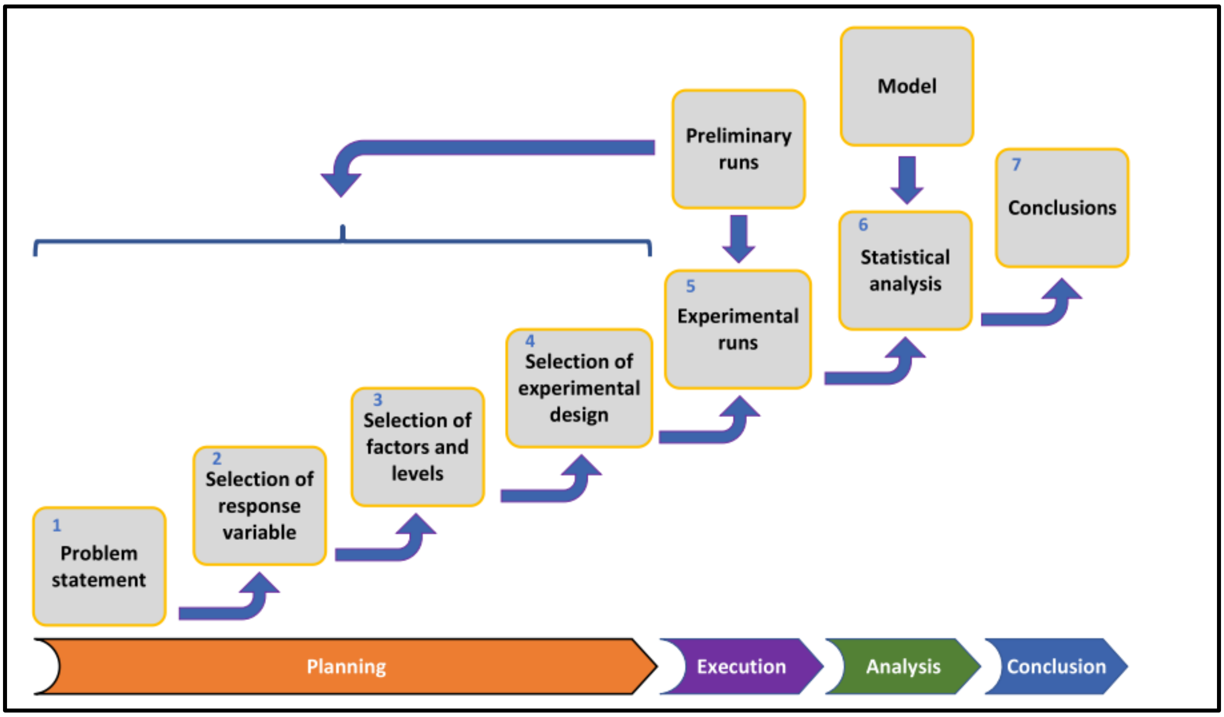

Figure 3. Steps in the DOE methodology. Source: [2]

Figure 3 depicts these steps within the aforementioned workflow, but it should be emphasized that the actual realization of such a methodology heavily depends on the type of problem as well as the targeted kinds of conclusions and objectives.

5.2 DOE for LIBs

In the context of LIBs, DOE methodologies have already been used to study many different subjects, that would go beyond the scope of this Deliverable in all their details. Therefore, this Deliverable only provides a condensed overview on the most relevant ones with respect to the FASTEST project in the following subsections.

5.2.1 Battery ageing

Studies related to battery ageing differentiate between calendar ageing which is related to the SEI build-up and cycling ageing, which is affected by SEI growth, lithium plating, volume changes and degradation effects in the electrodes. Electric current, temperature, and State of charge (SOC) and related quantities are usually considered as factors for the DOE in cycling aging, cf. [3]. The responses are defined by capacity and power fade. Most studies identify temperature and SOC as the main factors for capacity fading. In previous work focused on a D-optimal design, both calendar and cycling degradation modes could be combined into an empirical ageing model [4].

5.2.2 Energy Capacity

Few studies also investigated the relation of physical factors like particle sizes, electrode thickness, volume fraction of the active material and C-rate as factors on the specific energy and specific power as responses of interest. In previous work using a graphite / LFP chemistry, optimal power conditions are achieved if electrode thickness is less than 30 µm and the C-rate is equal to 5C. For optimal energy, particle size should be less than 40 nm, electrode thickness between 75 and 100 µm, and the volume fraction of the active material should range from 0.4 to 0.6 [5].

5.2.3 Formulation

DOE studies related to formulation consider different mixtures of components for electrolyte and electrodes and responses like discharge capacities, capacity retention and other cell performance indicators such as thermal conductivity. While most studies focus on the cathode chemistries and their optimal component mixture, several different designs have been used to arrive at such conclusions. For example, Rynne at al. [6] have studied the formulation with respect to active material, conductive additives, and polymer binder via d- and I-optimal designs.

5.2.4 Thermal Design

Thermal design studies aim at optimizing the temperature rise or related response quantities like total energy release or temperature of cooling plates. For that purpose, factors like mass of phase change material, thermal conductivity of paraffin copper composite and the rate of water flow are considered. A previous analysis concluded that all of the aforementioned factors have a significant influence on temperature rise while the most important one is the mass of phase changing material [7].

5.2.5 Model Parametrization

Due to the high need for fast and reliable parametrization of several for several types of models in the context of LIBs, DOE methodologies have also been used for parameter estimation and identification. For this purpose, different types and amounts of parameters have been studied in order to find optimal designs for parameter estimation usually based on a voltage response. A common approach is to investigate fisher-based optimality criteria in order to maximize the identifiability of parameters and reduce the time required for parametrization, cf. [8], [9].

As the FASTEST project aims at a time and cost reduction during testing using a hybrid testing platform and a high ratio of virtualized test, it was determined collaboratively, e.g. with partners from WP3: "Advanced battery aging and performance modelling", that these goals can be supported by a model-based DoE that aims at fast and reliable model parametrization. Therefore, the following subsection focuses on DOE methodologies as described above in Section 5.2.5.

5.3 DOE within FASTEST

After many iterations of presenting, discussing and evaluating different ideas, the FASTEST team was able to gather several ideas and directions regarding DOE methodologies, that are specifically tailored for the projects KPIs, while still leaving enough room and flexibility for future adjustments that may be needed. One of the main challenges of the FASTEST projects will be to tailor and optimize the resulting workflow for the wide range of different use-case that are covered within the project as described in Section 4. Additionally, a novel methodology based on Machine Learning is introduced that provides potential to speed up this workflow tremendously in several aspects and therefore pushing it further beyond the state of the art in the upcoming stages of the project.

As described before, the focus herein remains on DOE methodologies aiming at a fast and reliable model parametrization for efficient virtualization of tests. The reader is referred to previous work, e.g. in Deliverable D3.1 "Multiscale high fidelity modelling paradigm for physical testing virtualization", for an in-depth perspective on the different modelling approaches within FASTEST as well as the high need for a reliable parametrization of these models. Figure 4 outlines the different contributions that the proposed DOE methodologies can provide in this procedure.

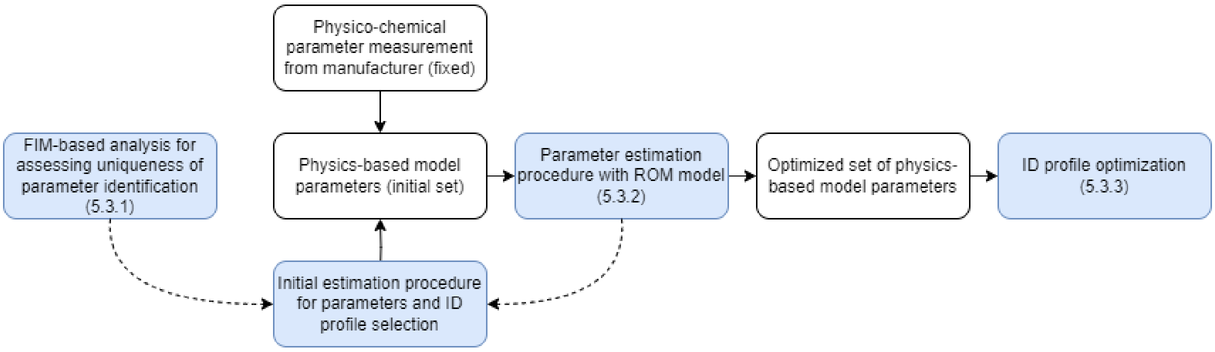

Figure 4. Proposed DOE workflow for parameter estimation and ID profile optimization.

In the following parts of this Deliverable, an in-depth explanation of the different DOE elements highlighted in Figure 4 is presented.

5.3.1 Development of model-based DOE methodology for assessing uniqueness of parameter identification

Electrochemical model of the battery cell (Newman inspired [10] pseudo 2D model [11], see Figure 5) inherently consists of number of physically based parameters that need to be determined during the parametrization procedure. These parameters range from geometry and structure properties of the cell (electrode and separator), morphology of the electrode material (e.g., particle size distribution), transport, electrical, thermal properties of electrolyte and electrode material.

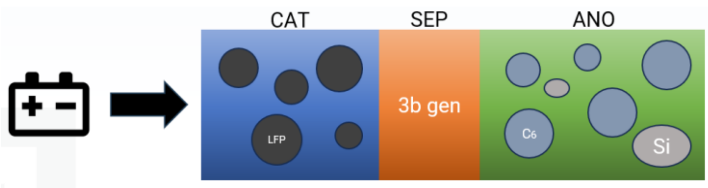

Figure 5. Schematic representation of electrochemical model domain for the 3b generation battery used in the first stage of the FASTEST project.

After the parametrization procedure is completed and model is validated against the experimental results, the question arises how uniquely a certain parameter is defined and how does the measurement settings and measuring protocol impact the uniqueness of parameter identification. To answer this question, the Fisher information approach was employed.

Fisher information is the centerpiece of all analyses performed. It indicates how much information an observable random variable, or in the case of a data set, a data point, carries about an unknown parameter vector θ. This can also be used in other ways: If we know the FIM, we can determine which unknown parameters in the parameter vector θ cannot be uniquely determined with the data set at hand [12]. In the analysed case, the unknown parameter vector θ represents the vector of the calibration. Mathematically, we can write down the definition of the FIM for the calibration parameters with Gaussian errors as follows:

$$FIM(U,\theta) = \frac{\partial f(U,\theta)}{\partial\theta}^{\mathsf{T}} \frac{\partial f(U,\theta)}{\partial\theta}$$

Where U is the observed outcome of the model at hand, θ is the aforementioned vector of calibration parameters and f is the function of the model.

Each individual element in this matrix carries different information about the parameters and their interdependence (see Figure 6). Diagonal elements represent the certainty of the determination of the calibration parameter, i.e., the inverse of the error in calibration parameter value, therefore a higher value here means a lower error.

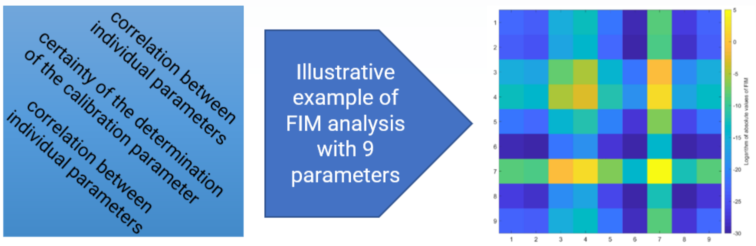

Figure 6. Schematic representation of the meaning of the diagonal and non-diagonal elements of the FIM matrix (left) and illustrative example of FIM matrix with 9 parameters (right).

On the other hand, the non-diagonal elements represent the correlation between the individual parameters. High values here mean that there is a high probability that the two parameters are barely separated from each other, that they are strongly interdependent and therefore cannot be well defined separately. However, in the case that the diagonal values are not high for all calibration parameters, this could also mean that this is only an effect of the higher diagonal value of the parameter with which the mixed partial derivative of the second order is formed. This can also be explained with an n-dimensional space parabola, where n is the number of calibration parameters. The FIM actually represents the derivative of the curvature of the n-dimensional surface. This means that if there is a significant gradient in the direction of one calibration parameter, there is a high probability that this will affect the gradients in the neighbouring directions if the n-dimensional curve is continuous and twice continuously differentiable. Therefore, these non-diagonal elements only indicate the independence or interdependence of the parameters.

This is confirmed or refuted by the FIM decomposition. Mathematically, the decomposition stands for the kernel calculation. Even without looking at the kernel itself, one can already tell a lot about the unique determination of the calibration parameters by simply looking at a rank of the kernel. As a general rule of thumb, the higher the rank, the more pronounced the inter-correlation between the parameters. However, a kernel with a low rank is a necessary but not sufficient condition to obtain an optimal quality of fit for a given set of experimental data while uniquely determining all calibration parameters. Theoretically, one could obtain the kernel of the FIM with rank zero, but the quality of fit would be poor, e.g. due to the modelling basis not being detailed enough or due to the fact that the optimisation gets stuck in a local instead of a global minimum. On the other hand, the kernel of the FIM could be obtained with a high rank, but the parameters would be almost uniquely determined and the intercorrelation between the parameters would be small but not zero, e.g. due to a non-Gaussian measurement error, measurement uncertainties or due to the suboptimal parameterisation of the model.

Besides the kernel, several so-called optimalities can be extracted from the calculated FIM. These optimality criteria bring additional information that can further maximise the efficiency of data collection in scientific experiments. Each optimality criterion reflects different aspects of the precision and efficiency of parameter estimation. The choice of optimality criterion depends on the specific goals and constraints of the experiment. The following optimalities were implemented to further support the FASTEST project's goals, namely:

- D-optimality, which is calculated from the determinant of the FIM,
- E-optimality, which is calculated from the minimal value of the eigen values of the FIM,
- T-optimality, which is calculated from the trace of the FIM.

Therefore, the experiment is for example D-optimal if the value of the D-optimality is minimized.

To conclude, with the aim of obtaining the best possible quality of fit and repeatability of the calibration process, the optimisation procedure should satisfy modelling constraints, while experimental data should provide enough information about the calibration parameters to enable unique the parametrisation of the model. Even though the latter is highly dependent on the modelling basis, a well-defined design of experiments could provide (if physical constraints do not prevent such type of excitation) a data set containing sufficient information about all calibration parameters of the model.

Preliminary results of the implemented methodology:

The proposed model-based DOE methodology for assessing uniqueness of parameter identification was implemented as a supporting library in the C-programming language. Calculation of the derivatives needed for calculation of the FIM was performed with the higher-order numerical derivation scheme to obtain accurate results. Besides the main result, i.e. FIM, the library also calculates various optimalities as mentioned above. To test the methodology, the developed FIM library was applied to the existing electrochemical model, which was set-up as a half-cell model and parametrized with thin NMC811 electrode since the measurements and parametrization of the FASTEST batteries were not yet available at the time of running these simulations.

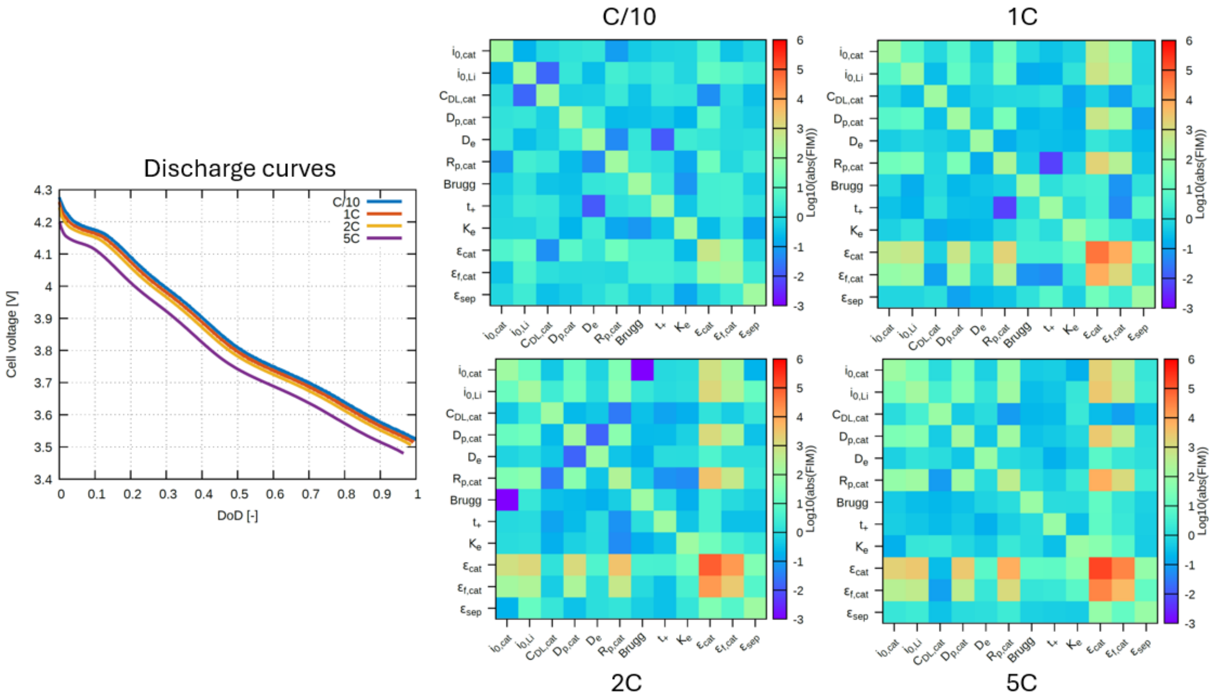

Figure 7. Preliminary results of the FIM analysis applied to the electrochemical model. Discharge curves of the thin NMC811 electrode (left), four FIM matrices corresponding to different C-rates (right).

Figure 7 shows the preliminary results of the FIM analysis applied to the half-cell electrochemical model with NMC811 as an active cathode material and Li-foil as a counter electrode. The FIM analysis was performed on the case of different discharge profiles at different C-rates, including C/10, 1C, 2C and 5C, shown on the left side of Figure 7. Four FIMs were calculated (shown on the right part of the Figure 7) for each C-rate. There are 12 electrochemical model parameters that were included in the analysis, namely the exchange current densities, double layer capacity, solid-phase diffusion constant, active particle size, Bruggeman coefficient, transference number, conductivity of the electrolyte, porosities of the cathode and separator and volume fraction of fillers in the cathode. Individual elements in the FIM are represented with a coloured square. The colour indicates the value of FIM element after applying log10 and absolute value to the calculated FIM, i.e. Log10(abs(FIM)), to better represent values due to several orders of magnitude difference between individual elements of the FIM (see colour bars in Figure 7).

A general observation of the FIMs in the Figure 7 reveals that values of the diagonal element feature relatively high values compared to the majority of the non-diagonal elements. The certainty of the determination of the calibration parameter and correlation between certain parameters increases with higher currents (shifting towards warmer colors in the colourbar). Furthermore, the porosity and volume fraction of the fillers in the cathode are the parameters with the highest certainty of determination. With increasing current, also the correlation between the two mentioned parameters and others, e.g. exchange current densities and particle size starts to increase. Low correlation, for example, can be identified between transference number and particle size, and between exchange current density at the particle/s surface and Bruggeman's coefficient. In the continuation of the FASTEST project, more detailed analyses will be performed.

5.3.2 Model-based DOE methodology for parameter estimation with reduced-order-models at cell level

In this section, the model-based DOE methodology for parameter estimation with reduced-order-models at cell level is explained. The main objective of this task is to present a workflow to accurately fit a certain number of model parameters which cannot be provided directly experimentally. This work is directly linked to WP3 of the project (advanced battery ageing and performance modelling), as the reduced-order-model at cell level is being developed there. The available physical performance and ageing testing have been defined in WP1 (specifications, requirements and use cases definition) according to the available testing standards of the literature for automotive, industrial and stationary applications. The test procedures are executed inside WP3 and are an input of this model-based DOE methodology (the profiles to be used). The profiles that can be used for parameter estimation (physically tested) are the followings at cell level: performance testing (capacity tests, pulse tests, qOCV tests, galvanostatic cycles at different current rates, thermal tests and use case application tests) and ageing testing (cycling and calendar). The methodology is presented in Figure 8.

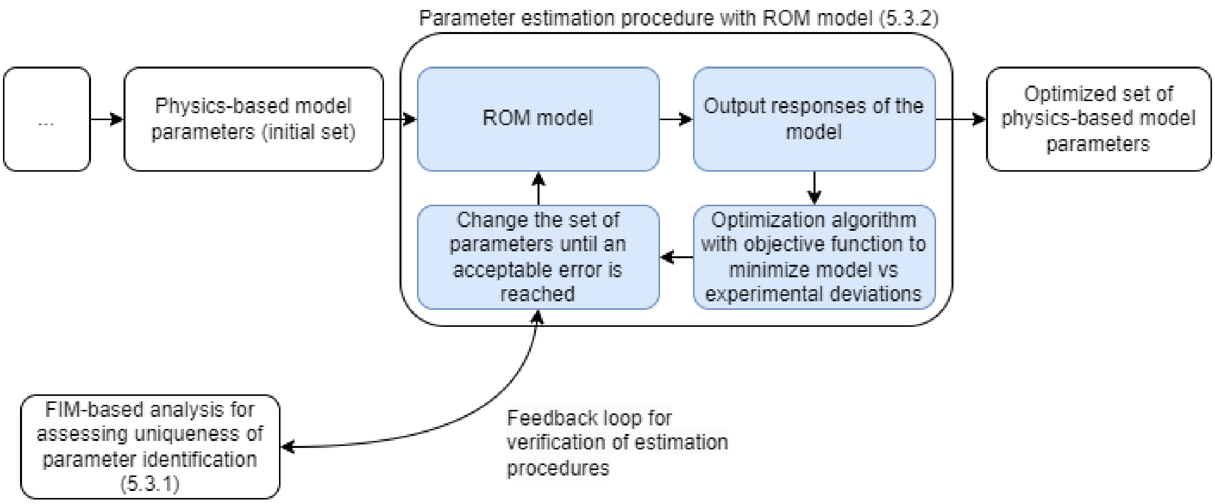

Figure 8. Model-based DOE methodology for parameter estimation with ROM at cell level.

The first step of this task is to define which parameters are provided experimentally and which of them need an optimization sequence to estimate them. This evaluation has already been done in T3.1 of the project, for which the partners involved in the modelling have requested to ABEE (the cell manufacturer) the parameter set to be defined. Based on that information, the parameters to be estimated are decided. The FIM analysis provides information on how uniquely the calibrated parameters are defined. Additionally, it provides a measure that can potentially define the optimal ID profile. After, the Reduced-Order-Model (ROM) is used in combination with an optimization algorithm to find the model parameters that minimize the difference between the simulated and experimental response of a measurable variable. Most commonly, this problem involves minimising the non-linear least square regression function, as expressed in equation 1:

$$F(\theta) = \min_{\theta} \sum_{i=1}^{N} \left(y_m(t_i) - y(t_i, \theta)\right)^2 \qquad (1)$$

where $y_m(t_i)$ is the measured variable and $y(t_i, \theta)$ is the model prediction with the parameter vector guess, θ. The optimisation algorithm stops when the difference reaches a minimum fitness value set by the user, which means an acceptable error of the model predictions.

5.3.3 ID profile optimization

Figure 9 schematically represents the potential methodology for optimizing input driving (ID) profile with the aim of maximizing the certainty of the determination of the calibration parameters with the aim of reducing experimental time for testing after parametrization is done, and therefore reducing also the costs.

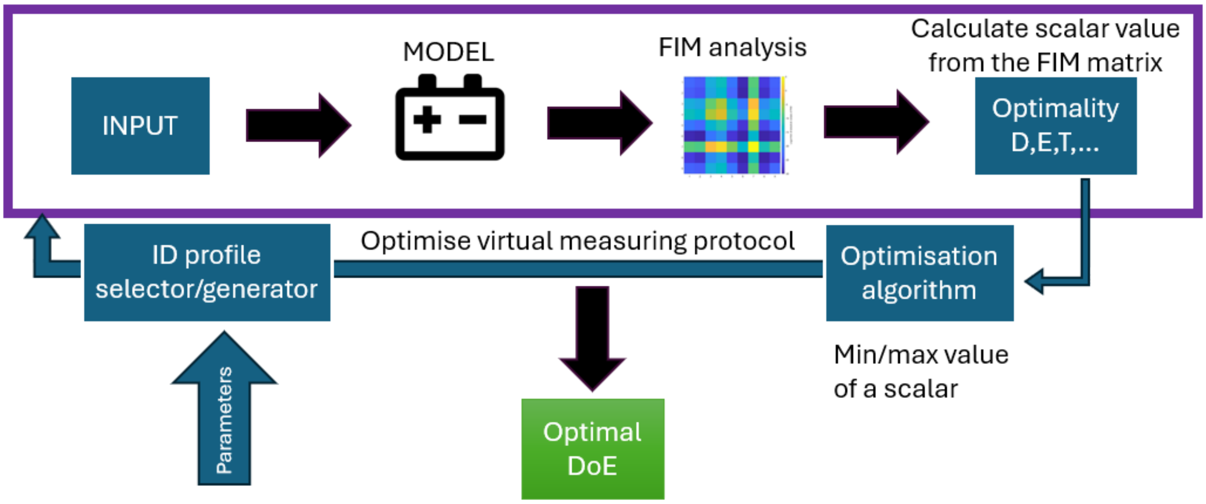

Figure 9. Proposed methodology for optimisation of the virtual measuring protocol.

The purple rectangle on the Figure 9 denotes the basis for the proposed methodology and includes Input, battery model, FIM analysis algorithm and calculation of Optimality. In the field of experimental battery characterization or battery modelling, the most common input would be the time-dependent current profile. For example, in Figure 7, a constant current over time was chosen for the analysis, however there are numerous current versus time profiles that are widely used in the field, e.g. simple cycling with (dis)charge currents, hybrid power pulse characterization (HPPC) or WLTP driving cycle, and many others. The challenge is in choosing the optimal profiles that provide the most information of the studied system, e.g. battery, and in the same time reduce the time needed to perform the experimental characterization.

The current profile is then applied to an already parametrized battery model, which as a result returns the time dependent voltage response (among other possible outputs of the model, e.g. state of charge, power, power loss, etc.). Then the FIM analysis is performed. Input current profile stays the same (refer to the Figure 7), only the selected model parameters are being perturbed. Selection of the parameters depends on the use case. Perturbation of the selected parameters affects the model output which is then fed into the Fisher information analysis library, which calculates the FIM. Examples of FIMs can be seen in Figure 7.

For the introduction of the optimization algorithm into the methodology, some sort of scalar value has to be extracted or calculated from the FIM which is NxN dimensional, where N is number of parameters in investigation, since it would not be feasible to optimize the entire FIM. These scalar values are called optimalities and are explained in the previous section and will serve as a measure for the optimisation algorithm.

Now that the basis (starting with input to the model and ending with an optimality value) denoted by the purple rectangle on the Figure 9 is established, the optimization algorithm can be applied on the basis. First, the decision has to be made on the optimality on which the design of experiment will be optimized. This again depends on the use case. The main task of the optimization algorithm is to take the value of selected optimality and provide a better set of calibration parameters that are responsible for selecting or generating new proposal for the ID profile, e.g. time dependent current profile. This is denoted by the "ID profile selector/generator" in Figure 9. The new ID profile is then selected/generated and fed back into the battery model as a new Input. The end result should be an ID profile that is optimal in terms of achieving optimal DoE and is defined with the parameters that select or generate the ID profile obtained by the optimization algorithm.

5.3.4 DOE methodologies based on Physics-Informed Neural Networks

As part of the screening process conducted in Task T2.1 of the FASTEST project, Physics-Informed Neural Networks (PINNs) were identified as promising and emerging option for pushing the aforementioned DOE methodologies beyond the state-of-the-art and further optimize and reduce experimental costs during battery testing.

PINNs represent a rather new form of machine learning, cf. [13], that combine neural networks with the principles of physics for solving partial differential equations (PDEs) and related continuum problems. These networks are trained to learn the underlying physics of a system by approximating and minimizing the corresponding residuals of differential equations, initial and boundary conditions instead of relying solely on large amounts of data to minimize the differences between the networks output and corresponding data. PINNs have been successfully applied to a wide range of problems in fluid dynamics, heat transfer, structural mechanics, and other fields where PDEs govern the behavior of physical systems. By integrating domain knowledge and constraints into the neural network architecture, PINNs can effectively capture complex nonlinear phenomena and can also be combined with noisy or sparse data.

After training in a generalized fashion over certain parameter ranges PINNs can be used for inference of simulation results in a matter of milliseconds. In a related approach, usually referred to as Operator Learning, such networks can be extended to generalize over discrete functional inputs - e.g., representing temporally or spatially varying boundary conditions – in order to learn a mapping between function spaces, i.e. an operator. This setup can also be trained in a physics-informed manner, explaining the notion of Physics-Informed Deep Operator Networks (PI-DeepONets) [14]. Due to their relatively small requirements regarding software and hardware environment, such networks are also feasible candidates for deployment on edge computing devices, e.g., in the context of a battery management system (BMS).

In the scope of the FASTEST project, classical PINNs or PI-DeepONets have been identified as potential surrogate models for the different types of models which are explained more thoroughly in previous work (cf. Deliverable D3.1). By generalizing over different (unknown) parameters or current profiles, they are of specific interest for the DOE methodologies developed in the FASTEST project. Figure 10 shows an exemplary architecture of a PI-DeepONet, which is trained to predict the Lithium concentration within a LIB-cell based on the governing equations of the Single-Particle-Model (SPM).

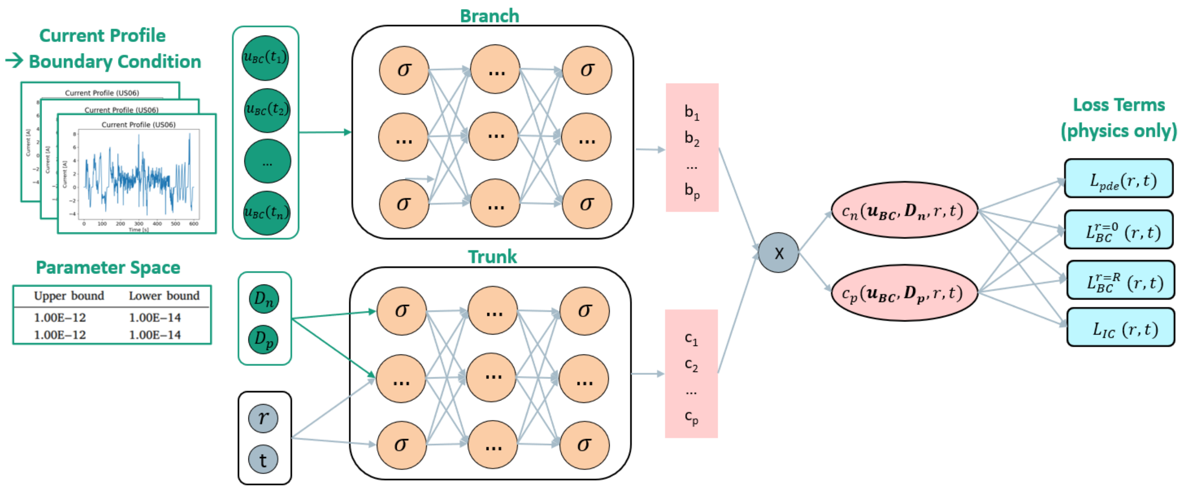

Figure 10. PI-DeepONet for Prediction of SPM solutions ($c_n(r,t)$ and $c_p(r,t)$) for different current profiles and diffusivities.

By training this network over a (pre-defined or randomized) set of current profiles (cf. "Branch" input in Figure 10), and a continuous parameter space (indicated for anode and cathode diffusivities in the "Trunk" input of Figure 10), this surrogate model can be used for parameter estimation in the same manner as indicated in Section 5.3.2.

Furthermore, after parameters are identified, this network can also be employed for the FIM-based assessment of parameter uniqueness as introduced in Section 5.3.1. This is specifically interesting as the required gradients for the FIM analysis can be approximated quickly by automatic differentiation (AD), the same technique used for approximating any physical gradients during the network training without the need for time-consuming numerical differentiation schemes.

In the follow-up tasks of WP2, this methodology will be investigated more thoroughly with respect to the different use case boundary conditions and objectives defined in Section 4 of this Deliverable.

6. Conclusion

This deliverable provides in the first part the formulation of the objectives, success criteria and boundary conditions of the three use cases considered in FASTEST: automotive, stationary energy storage and off-road mobile devices. The second part of the deliverable presents and evaluates the proposed model-based DoE approaches and methodologies to be applied in the upcoming stages of the FASTEST project.

In Section 4, a thorough investigation of the presented use cases has been conducted in terms of battery testing boundary conditions. The considered testing procedures have been divided between those that need to be considered distinctively for each use case and those that are common among all use cases. Most notably, exemplary current profiles were presented for each use case which will be of high significance for the aging testing and related modelling activities throughout the rest of the project.

In Section 5, the model-based DOE methodology for parameter estimation with reduced-order-models at cell level was presented. The main objective of this part is to propose a workflow that is able to accurately determine physics-based model parameters effectively enabling virtualization of tests in the hybrid testing platform developed within FASTEST.

The Fisher information approach was developed to answer the question how uniquely a certain parameter is defined in the parametrized model and how does the measurement settings and measuring protocol impact the uniqueness of parameter identification. The theory behind the FIM approach was presented and initial results of the approach were shown. The results revealed an important insight into the certainty of the determination of the chosen calibration parameters and the correlation between the individual parameters. Based on this approach, an innovative methodology was proposed to define the optimal design of experiment, which can reduce the time and costs for experimental testing further after the initial model parametrization is done.

Although, the computationally efficient electrochemical models will be used in the FASTEST project, they might still feature high combined computational times when searching for optimal DoE. To further push the DOE methodologies beyond the state-of-the-art and further optimize and reduce experimental costs during battery testing, Physics-Informed Neural Networks (PINNs) were identified as promising and emerging option due to their high versatility and extremely fast inference times in the order of milliseconds.

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