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FASTEST

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

Deliverable D4.3: Integration & optimisation of battery AI-powered battery multi-domain toolchain cell to system level.

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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 generalized 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, virtualized 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 data driven models able to substitute physical characterization 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
ASIL	Automotive Safety Integrity Level
DoE	Design of Experiments
DT	Digital Twin
EIS	Electrochemical Impedance Spectroscopy
FMI	Functional Mock-up Interface
ISO	International Organization for Standardization
HARA	Hazard Analysis and Risk Assessment

HIL	Hardware in the Loop
LIMS	Laboratory Information Management Systems
NMC/Si-C	Nickel-Manganese-Cobalt/Silicon-Carbon
OPC UA	Open Platform Communications Unified Architecture
PINN	Physics-informed neural network
RUL	Remaining useful life
SAE	Society of Automotive Engineers
SOH	State of Health
TRL	Technology Readiness Level
WP	Work Package

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1. EXECUTIVE SUMMARY

This deliverable, D4.3, explains how the high-fidelity, AI-powered multi-domain toolchain for testing the safety and reliability of virtual batteries was developed and enhanced as part of Work Package 4 (WP4) of the FASTEST project [1]. This report focuses on the critical step of expanding the toolchain from individual cell-level models to a fully integrated and optimised system-level platform. It builds on the basic architecture from T4.1 and the model development from T4.2 [2]. Combining AI-powered diagnostic tools with physics-based multi-scale modelling is a big step forward in how we test battery systems.

Current methods for testing battery safety and reliability are resource-intensive and time-consuming. They involve a lot of physical testing and trial-and-error methods, but don't fully understand how complex multi-physics phenomena work [3]. The primary objective of this work is to systematically integrate several subsystems, including advanced ageing models from WP3, to create a coherent framework for conducting complex safety and reliability analyses, such as Failure Mode and Effects Analysis (FMEA), hazard analysis, and risk assessments, on complete battery modules and packs. This integrated environment demonstrates how mechanical, thermal, and electrochemical processes interact at the system level [4].

An essential part of this phase is optimising artificial intelligence (AI) and machine learning (ML) algorithms to improve their performance, enabling system-level diagnostics and prognostics to be more accurate and faster. The toolchain's established and enhanced connections with the broader FASTEST ecosystem [5], which includes the Digital Twin (WP5) and the hybrid testing platform (WP6), ensure that data flows smoothly and that all components work together through standard protocols, such as the Functional Mock-up Interface (FMI). This report outlines the comprehensive validation and verification processes employed to ensure the toolchain was accurate, reliable, and compliant with key industry standards, including IEC 61508 Ed. 2.0 and ISO 26262:2018. The successful integration and optimisation described here are a significant step towards the FASTEST project's goal of accelerating battery research and development by creating a robust, validated, and interconnected virtual testing platform.

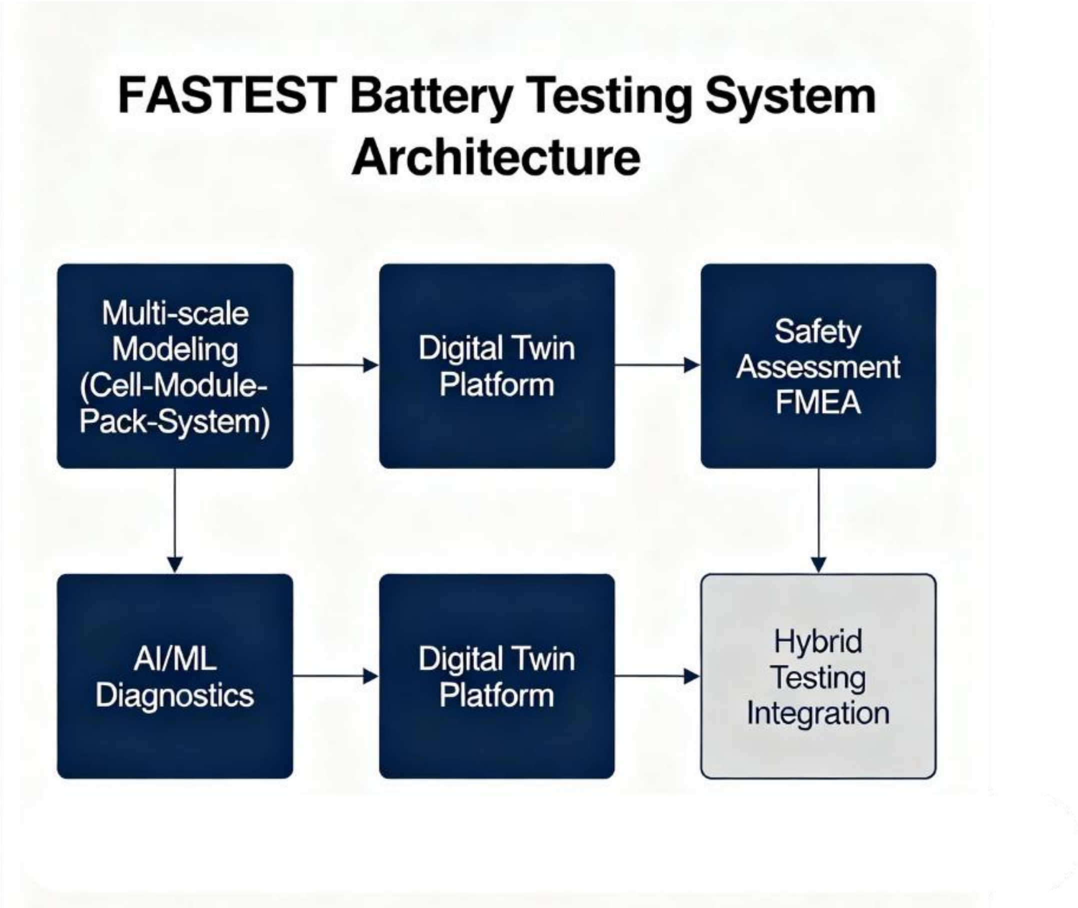

Figure 1 - FASTEST System Architecture - Integrated Multi-Domain Toolchain

2. Introduction

By developing a fast-track hybrid testing platform that combines virtual and physical testing, the FASTEST project aims to transform battery system research and development. Work Package 4 (WP4), which is devoted to providing a novel toolchain for the virtual testing, analysis, and validation of battery safety and reliability, is a crucial part of this effort. From the cell to the fully integrated pack, this toolchain is designed to be a high-fidelity, modular computational environment capable of evaluating battery systems at various hierarchical levels [6].

Current battery testing methodologies face significant limitations, including high resource consumption, time-intensive processes, and a limited understanding of the underlying multi-physics phenomena that govern performance and degradation. The development of hybrid testing platforms, which intelligently combine physical and virtual experimentation, represents a paradigm shift toward more efficient and comprehensive assessment approaches. Within this paradigm, Digital Twin (DT) technologies are pivotal, enabling the real-time integration of physical and virtual testing environments and providing unprecedented capabilities for battery system optimisation and predictive maintenance [7].

This document, D4.3, details the activities of Task 4.3: "Optimisation and integration to the system level." This task marks the critical shift from creating standalone, high-fidelity models (T4.2) to incorporating them into a comprehensive, system-level simulation and analysis framework. The primary goal is to examine the different subsystems and innovative concepts to prolong battery life and lower maintenance expenses through virtual assessment. The integration process involves scaling up cell-level models and incorporating system-level effects such as inter-cell variability, thermal management, and electrical balancing. Emphasis is placed on performing system-level hazard analysis, risk assessments, and Failure Mode and Effects Analysis (FMEA) to identify and address potential vulnerabilities before physical prototyping [8].

This report describes the development of robust interfaces with the Digital Twin (WP5) and the Laboratory Information Management System (LIMS) of the hybrid platform (WP6), as well as the optimisation of AI-powered algorithms for system-level applications. This guarantees smooth data transfer and co-simulation capabilities, which are essential components of the FASTEST hybrid testing concept. Additionally, the validation and verification procedures for the integrated toolchain are described, ensuring its dependability and conformity to global safety regulations [9].

The Table 1 summarises the core technical pillars of the WP4 toolchain, aligning them with the key standards and foundational scientific literature that underpin their development.

Toolchain Pillar	Core Methodology	Key Enabling Standards
Multi-Scale Modeling	Hierarchical integration of physics-based models from cell (e.g., P2D) to pack level, capturing coupled electro-chemo-thermo-mechanical effects.	N/A
Safety & Reliability	Virtual Failure Mode and Effects Analysis (FMEA/FMMEA), hazard analysis, and simulation of critical failure events (e.g., thermal runaway).	ISO 26262:2018 , IEC 61508 Ed. 2.0, SAE J2464:2021
AI-Powered Prognostics	Hybrid approach combining data-driven models (LSTM, Ensembles) with Physics-Informed Neural Networks (PINNs) for SOH/RUL prediction.	ISO 26262-6 (Software)
System Integration	Integration with a Digital Twin and hybrid testing platform via standardized, interoperable interfaces for co-simulation and data exchange.	FMI 2.0/3.0 , OPC UA

Table 1 - Alignment of FASTEST Toolchain Pillars with Key Standards and Foundational Literature

3. Advanced Multi-Scale Modelling and Integration Framework for Battery System Safety and Reliability

The WP4 toolchain is built on a modular, service-oriented framework designed to integrate seamlessly with a wide range of external platforms. This architecture facilitates the combination of different modelling methods, such as high-fidelity physics-based models and data-driven surrogates, each designed to examine a distinct aspect of how batteries function under various conditions. This modularity makes it easy to adapt to changing times, as battery technologies and research problems evolve.

3.1 From Cell to System: A Multi-Scale Integration Approach

The toolchain employs a multi-scale modelling hierarchy, initiating with granular fidelity at the cellular level and gradually integrating these models into more extensive module and pack-level frameworks. This hierarchical approach is necessary to strike a balance between the ease of computation and the accuracy of prediction.

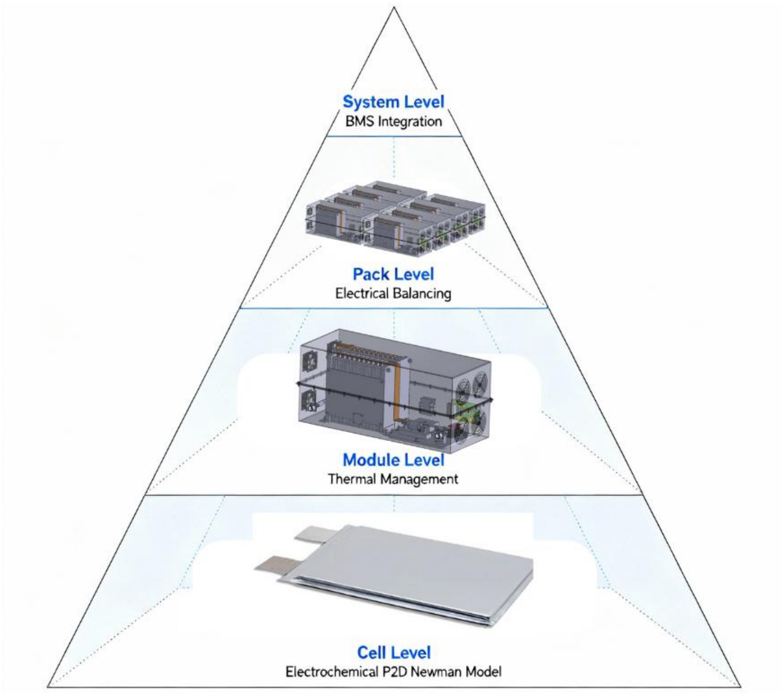

Figure 2 - Multi-Scale Battery Modeling Hierarchy - Cell to System Integration

Cell-Level Fidelity

The toolchain utilises advanced electrochemical, thermal, and mechanical models to simulate the fundamental processes that impact battery performance, degradation, and failure at the most detailed level. Electrochemical models derived from the Pseudo-Two-Dimensional (P2D) framework, initially established by Newman and associates, offer essential insights into lithium-ion transport and reaction kinetics [10]. These models are carefully parameterised with high-resolution experimental data to ensure a high level of predictive accuracy. They enable the examination of localised processes that are critical precursors to cellular ageing and catastrophic failure, including lithium plating, electrode fracturing, and electrolyte decomposition [11]. The real breakthrough lies in linking these models together to demonstrate how different phenomena interact with one another. For example, how stress caused by intercalation (mechanical) affects reaction kinetics (electrochemical) and heat generation (thermal).

Integration at the Module and Pack Level

Detailed module and pack simulations use advanced upscaling methods to include cell-level models. The biggest problem with this upscaling is that it is costly to simulate thousands of high-quality cell models simultaneously. To solve this problem, the framework employs methods such as model order reduction and the creation of data-driven surrogate models to generate representations of individual cells that are both physically accurate and computationally efficient. This process takes into account critical system-level factors, such as balancing electricity, managing heat, inter-cell variability, and other complex interactions between systems [12]. Multi-scale modelling methods accurately capture these system-level dynamics, enabling the simulation of scenarios such as local failure propagation and the assessment of overall system resilience, and providing crucial insights for practical applications.

3.2 System-Level Optimisation for Performance, Safety, and Reliability

By combining models from the cell level to the system level, it is possible to optimise everything at once. The toolchain is designed to examine the entire system, making it faster, safer, and more reliable.

- Subsystem Analysis: The toolchain enables you to examine various subsystems and new ideas in depth, assessing their impact on the battery system's lifespan and maintenance costs. Advanced degradation modelling techniques, which take into account both calendar and cycle ageing effects, provide a comprehensive understanding of how long a battery will last under various usage conditions.
- Enhancing System Architecture and Function: The toolchain can be used to enhance system design and operational strategies by analysing large datasets from battery systems in various operational contexts. This makes it easier to use techniques for reducing risk and doing maintenance ahead of time. Design of Experiments (DoE) methods enable the systematic improvement of battery testing protocols and operational parameters.
- Integration of the Lifecycle: The toolchain can handle two-way data flows, allowing real-time operational data to be used for calibrating and validating models. The simulation results are then sent to the Digital Twin and hybrid testing platforms, allowing for scenario analysis and closed-loop co-simulation throughout the entire life cycle of the battery system [13].

4. Safety and Reliability Assessment Methodologies

One of the most essential features of the integrated WP4 toolchain is its ability to do thorough safety and reliability checks at the system level. This is achieved by utilising well-established engineering methods in the virtual world, which enables the identification and mitigation of risks early on, well before physical prototypes are created.

4.1 FMEA, Hazard Analysis, and Risk Assessment

The toolchain enables thorough safety and reliability tests on models of the integrated battery system. The goal is to identify hidden failure modes and assess the associated risks before entering the physical prototyping stage. This virtual safety assessment marks a significant change in the engineering workflow. It aligns with the V-model development process, which is at the heart of standards like ISO 26262. It is possible to identify and rectify a critical failure mode during the virtual system design phase, rather than during costly and potentially hazardous physical pack-level abuse testing.

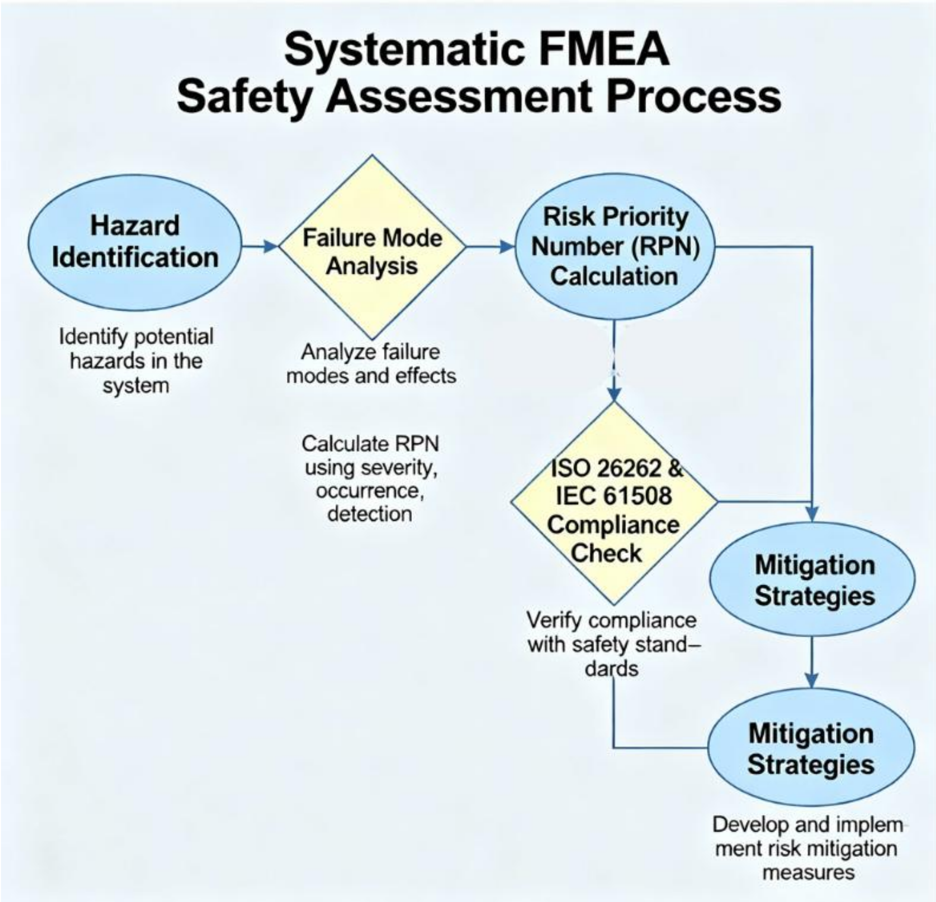

Figure 3 - Safety and Reliability Assessment - FMEA Workflow with Standards Compliance

- Failure Mode and Effects Analysis (FMEA): A system-level FMEA is done on important parts as part of T4.3. To deal with the unique failure modes that come with electrochemical energy storage systems, such as thermal runaway propagation, internal short circuits, and control system malfunctions, battery-specific FMEA methods are used. For a more in-depth analysis, the toolchain also supports Failure Mode, Mechanisms, and Effects Analysis (FMMEA). This is a more thorough method that links failure modes to their physical or chemical causes, giving you a better understanding of what caused the failure [14].

- Risk Assessment and SIL Allocation: The FMEA process follows the IEC 61508 standard by systematically identifying possible failure modes, determining their impact on the system, and categorising them based on severity, frequency, and ease of detection. To choose a Risk Priority Number (RPN), these variables are combined. The RPN is a structured method for ranking risks and determining which actions to take first to mitigate them. This method ensures that all assumptions can be traced back and that the Safety Integrity Level (SIL) allocation rules in IEC 61508 are adhered to.

4.2 Simulating Failure and Degradation

The toolchain's integrated modelling environment captures the complex interactions between mechanical, thermal, and electrochemical processes that lead to battery ageing and failure.

Critical Event Simulation

The toolchain utilises high-fidelity physics-based modelling to predict critical events, such as thermal runaway, internal short circuits, and structural failure, in both standard and abusive operating conditions. Coupled multi-physics methods are employed to model the initiation and progression of these failure modes. Thermal runaway is the primary focus, and it requires a deep understanding of how heat is generated, how gas evolves, and how heat is transferred between cells. We verify the results of these simulations against experimental data to ensure their accuracy.

Advanced Ageing and Degradation Models

The toolchain takes into account the effects of capacity fade, impedance growth, and both calendar and cycle ageing, all of which were modelled in WP3. These mechanistic ageing models provide a fundamental understanding of how materials break down, including the formation of the solid electrolyte interphase (SEI), the loss of active material, and the decrease in lithium inventory. These models are necessary for predictive diagnostics throughout the battery lifecycle because they are based on both lab and field data.

4.3 Standards Compliance

The toolchain's methods and processes are designed to adhere to the relevant international standards for battery safety and reliability. This ensures that the virtual testing and assessment workflows yield results that are useful for obtaining certification and approval from the government.

- ISO 26262 - Functional Safety: It is essential to follow ISO 26262:2018 for cars. The standard outlines structured methods for conducting hazard analysis, risk assessment (HARA), and determining Automotive Safety

Integrity Levels (ASILs) for battery management systems and other critical electronic components, which are crucial for safety [15].

- IEC 61508 - Functional Safety of Electrical Systems: IEC 61508, Edition 2.0, is the primary standard for functional safety. It establishes the rules for ensuring that electrical, electronic, and programmable electronic systems are safe. The toolchain's assessment workflows utilise its concepts regarding SIL determination and safety lifecycle management [16].
- SAE J2464 - Battery Abuse Testing: The Society of Automotive Engineers (SAE) J2464:2021 standard provides guidelines for safely and correctly testing rechargeable energy storage systems. The virtual test scenarios created in the toolchain are designed to align with the physical testing protocols outlined in this standard. This ensures that virtual validation can serve as a valid replacement for specific physical tests [17].

4.4 System level FMEA analysis for Toolchain and battery system

Failure Mode and Effects Analysis (FMEA) has been applied at the system level to both the integrated multi-domain toolchain and the battery system. This ensures that latent risks are systematically identified, quantified, and addressed early in the design process. The dual-level approach provides a comprehensive framework: assessing the reliability of the toolchain as a predictive and monitoring platform and evaluating the safety-critical aspects of the battery system under real-world operating conditions.

This system-level FMEA aligns with IEC 61508, ISO 26262, and SAE J2464 standards, ensuring compliance with international safety and reliability requirements. Each failure mode is assessed against severity, occurrence, and detection to calculate a Risk Priority Number (RPN), which guides prioritization of mitigation measures. The combined assessment strengthens predictive diagnostics, extends system lifetime, and enhances operational safety.

4.4.1 Toolchain level FMEA analysis

The toolchain-level FMEA identifies risks that affect data integrity, integration with external systems, predictive accuracy, and real-time monitoring capability. Addressing these risks ensures that the toolchain functions as a reliable virtual testing and monitoring environment for battery safety and reliability analysis. The results of this analysis are summarised in Table 2: Toolchain-level FMEA.

Failure Mode	Cause	Effect	S	O	D	RPN	Current Controls	Recommended Actions
Model Drift / Inaccurate Predictions	Insufficient calibration, limited datasets, changing operating conditions	Incorrect prognostics (RUL, fault detection), leading to misguided maintenance actions and reduced trust in DT outputs	9	5	4	180	Calibration workflows, validation against lab/HIL data, cross-model comparison	Expand calibration datasets, apply continuous learning, uncertainty quantification, automated alerts for drift

Integration Failure (Toolchain ↔ BMS ↔ WP3 Models)	Version mismatch, interface incompatibility, API changes	Toolchain unable to communicate with BMS or WP3 outputs, resulting in loss of functionality or incorrect system optimization	9	4	3	108	Version control, integration tests, CI/CD pipelines	Define formal interface contracts, use automated integration tests, continuous integration
Data Loss or Corruption	Network disruptions, EMI, protocol mismatch, storage failures	Incomplete or corrupted datasets leading to poor prognostics and incorrect DT calibration	8	4	4	128	Checksums, retries, redundant storage, error correction protocols	Implement QoS protocols, redundant data paths, hardened communication protocols
Algorithm Bias / Misclassification	Imbalanced training data, poor feature engineering	False positives or negatives in anomaly detection, leading to unnecessary maintenance or missed faults	8	5	4	160	SMOTE/oversampling, cross-validation, confusion matrix monitoring	Improve dataset balancing, incorporate explainable AI methods, regular retraining
Latency / Real-Time Constraints	Insufficient computational resources, inefficient algorithms	Delayed fault detection or missed real-time alarms, undermining safety	9	3	4	108	Performance benchmarks, real-time HIL testing, code optimization	Optimize algorithms, allocate dedicated hardware, monitor latency continuously
Uncertainty Handling Failure	Lack of robust methods to quantify prediction uncertainty	Overconfidence in predictions, poor decision support	7	4	3	84	Error bounds, RMSE/MAE tracking, calibration plots	Implement Bayesian methods, prediction intervals, confidence scoring
Software Bug / Control Logic Error	Poor code quality, insufficient testing	Wrong alarms, missed detection, unsafe actions	9	4	3	108	Code reviews, HIL testing, automated unit/integration tests	Adopt CI/CD, enforce coding standards, conduct safety audits (IEC 61508 alignment)

Table 2 - Toolchain-level FMEA

4.4.2 Battery system level FMEA

The battery system-level FMEA captures degradation phenomena, ageing mechanisms, and safety-critical events across cells,modules, and packs. It highlights how electrochemical, thermal, and mechanical factors interact to influence capacity fade, impedance growth, thermal runaway risk, and other hazards. By addressing these risks early through virtual testing, the toolchain improves predictive diagnostics and informs safer system design. The detailed outcomes are presented in Table 3: Battery system-level FMEA

Failure Mode	Battery Type	Use Cases	Test Level	Cause	Effect	S	O	D	RPN	Recommended Actions
Capacity Fade (accelerated)	Gen3, Gen4	Automotive, Stationary, Off-road	Cell, Module	Electrode degradation, SEI growth, cycling	Reduced usable capacity, range loss, reduced runtime	7	6	4	168	Periodic capacity tests, reference cycles, model calibration; materials/processing improvements
Lithium Plating	Gen3	Automotive, Off-road	Cell	Fast charge at low temp, high-rate charge	Capacity loss, increased impedance, internal shorts risk	9	5	6	270	Fast-charge tests at low temp, post-mortem analysis, detect via EIS and coulombic efficiency
Internal Short / Dendrite Penetration	Gen3	All (esp. Automotive)	Cell, Module	Dendrite growth, manufacturing defects	Sudden voltage drop, local heating, thermal runaway initiation	10	4	7	280	Abuse tests, CT scans, thermal imaging, enable early detection algorithms and separator improvements
Thermal Runaway Propagation (pack-level)	Gen3, Gen4	Stationary, Automotive	Module/System	Cell thermal event, poor thermal management, venting	Cascading cell failure, fire, catastrophic damage	10	3	5	150	Pack abuse tests, thermal imaging, calorimetry, improve thermal barriers and layout
Thermal Management Failure	Gen3, Gen4	Automotive, Stationary	Module/System	Pump/fan failure, coolant leak, controller error	Localized overheating, accelerated ageing, safety risk	9	4	5	180	Thermal cycling, cooling-off tests, redundancy in thermal system, monitoring

Table 3 - Battery system-level FMEA

5. Artificial Intelligence and Machine Learning Techniques

A key innovation of the WP4 toolchain is the strategic integration of AI and ML, which enhances safety and reliability assessments by enabling more accurate predictions of potential outcomes [18]. As the toolchain scales to the system level, these methods are improved to handle the additional complexity and data volume associated with full battery packs.

5.1 System-Level Predictive Diagnostics and Risk Analysis

The toolchain enables system-level predictive diagnostics and risk assessment by integrating advanced machine learning techniques with physics-informed modeling. As illustrated in Figure 4, the architecture is designed to process heterogeneous time-series data and deliver accurate, interpretable predictions of battery health and operational risk.

Data Acquisition and Preprocessing

The pipeline begins with Input Data Streams, which include high-resolution measurements from integrated system simulations and operational logs under both nominal and abusive conditions. This comprehensive dataset ensures robust model training and generalization.

Supervised Learning Models

Three neural network architectures—Long Short-Term Memory (LSTM), Recurrent Neural Network (RNN), and Convolutional Neural Network (CNN)—are employed to capture complementary aspects of the data:

- LSTM networks model long-range temporal dependencies, mitigating vanishing gradients and enabling early detection of degradation trends [19].
- RNNs capture short-term dynamics, improving responsiveness to transient behaviors.
- CNNs extract localized patterns and spatial correlations from structured representations, enhancing fault detection capabilities [20].

These models operate in parallel, providing diverse feature representations that collectively improve predictive robustness.

Physics-Informed Neural Network (PINN)

To ensure physical consistency and interpretability, a Physics-Informed Neural Network integrates electrochemical constraints into the learning process. This hybrid approach mitigates physically implausible predictions and strengthens generalization under unseen conditions [21].

Ensemble-Based Aggregation

Outputs from the supervised models and PINN are consolidated through Ensemble Methods, such as random forests and gradient boosting machines. These techniques combine multiple weak learners to enhance predictive accuracy and provide interpretable decision boundaries, facilitating transparent risk assessment and actionable insights.

Predictive Outputs

The final stage generates two key indicators for system-level diagnostics:

- State of Health (SOH): Quantifies degradation and remaining useful life.

- State of Charge (SOC): Reflects current energy availability and charging status.

Design Rationale

The architecture prioritizes modularity and complementarity: direct data flow to each neural network enables specialized feature extraction, while ensemble aggregation ensures robustness and interpretability. PINN serves as a physics-based refinement layer, reinforcing reliability in safety-critical applications.

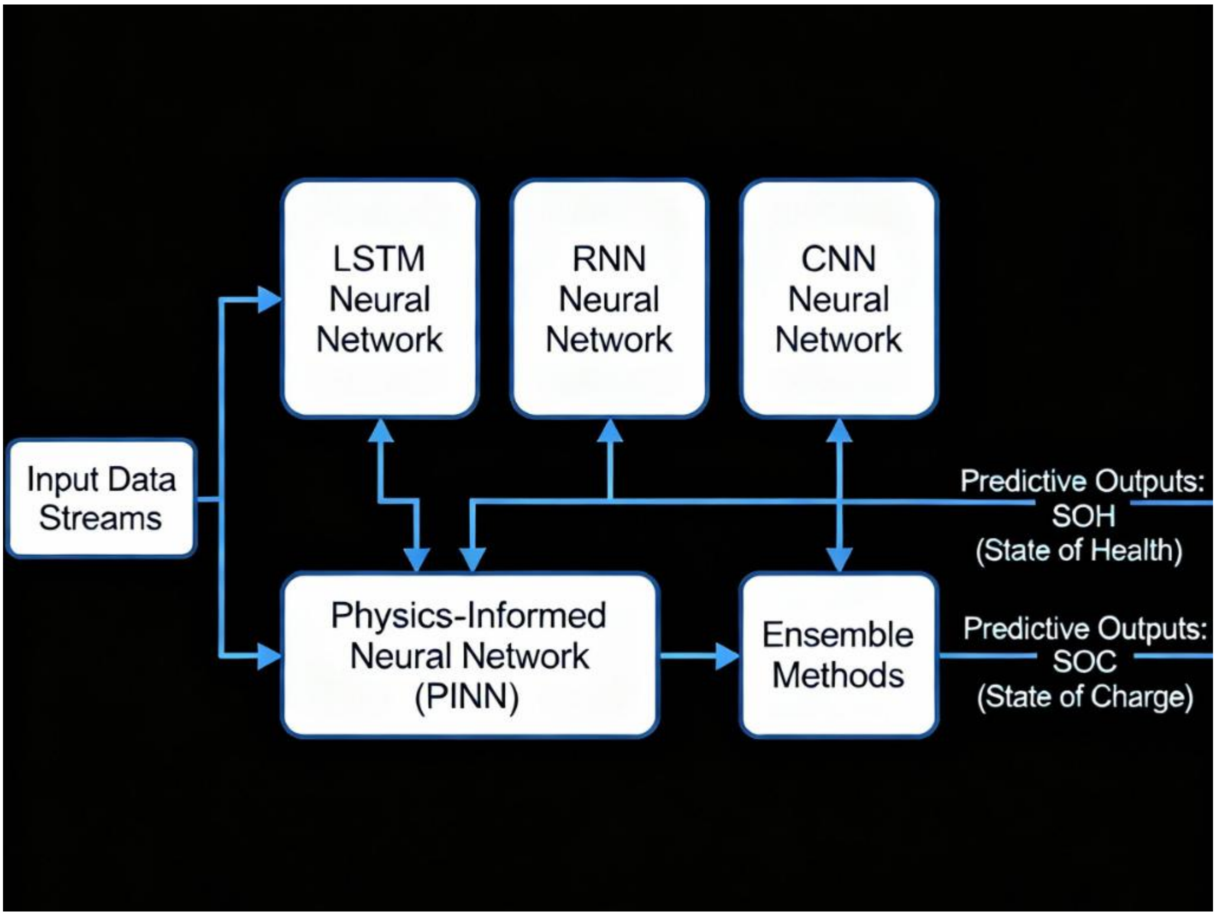

Figure 4 - AI/ML Framework - Battery Diagnostics and Prognostics Integration

5.2 Optimization and Adaptation of AI/ML Models

The toolchain extends beyond regular ML applications by utilising advanced and hybrid methods designed to address the challenges faced by battery systems.

- Unsupervised Learning: The toolchain employs unsupervised learning methods, such as clustering and anomaly detection algorithms, to identify unusual or previously unseen failure patterns in large operational datasets. This is especially useful for adapting safety models to address new threats that were not present in the original training data.
- Physics-Informed Neural Networks (PINNs): The combination of PINNs is a big step forward in battery modelling. One of the significant challenges in

utilising AI for battery management is obtaining high-quality training data that encompasses all possible operating conditions. This method solves that problem. Models that are only based on data often have a hard time applying what they learnt to situations they haven't seen before. PINNs mitigate this problem by incorporating physical laws (such as conservation of charge and electrochemical kinetics) directly into the training process of the neural network as a means to regularise it. Combining first-principles knowledge with data-driven learning reduces the need for large datasets and ensures that the model's predictions remain physically sound. This makes the model more generalisable and robust.

- Hybrid Model Integration: One important strategy is to use hybrid models that combine the physical accuracy of mechanistic models with the data-driven insights of AI/ML. This synergy enables the toolchain to make highly accurate predictions and work effectively with various battery chemistries and system architectures, thereby making virtual testing more reliable overall.

6. Interfaces and Integration with Digital Twin and Hybrid Testing Platform

A significant part of Task 4.3 is ensuring that the system-level, optimised toolchain functions effectively within the larger FASTEST digital ecosystem. This ecosystem comprises the Digital Twin (DT) developed in WP5 and the hybrid testing platform, which incorporates the Laboratory Information Management System (LIMS) from WP6.

6.1 Architectural Integration and Interoperability

The toolchain's architecture is fully compatible with the DT infrastructure, enabling thorough virtual validation, model co-simulation, and real-time, two-way data exchange. Standardised interfaces and communication protocols are necessary for interoperability, making this integration possible [22]. Choosing industry-backed standards over proprietary protocols is a strategic move that sets the FASTEST platform up for widespread use in industry and future growth. This method ensures that the parts of the toolchain can easily integrate into current commercial simulation workflows and factory automation systems. This makes it easier to transfer technology and make money from it.

- Standardised Interfaces: The toolchain utilises industry standards, including the Functional Mock-up Interface (FMI) and the Open Platform Communications Unified Architecture (OPC UA) [23]. The FMI standard facilitates co-simulation and the sharing of various modelling assets. For example, models from WP3 and WP4 can run as "virtual benches" on the WP6 platform. FMI establishes a container and an interface for exchanging dynamic models through a combination of XML files and compiled C code, rendering it a tool-agnostic standard for both model exchange and co-simulation.

- Communication Protocols: OPC UA is a secure, reliable, platform-independent, and service-oriented way for different systems to share data. In industrial settings, the toolchain, the DT, and the LIMS need to be able to communicate with each other in real time. This choice aligns with major industry projects, such as the VDMA and VDA working group, which is developing an OPC UA Companion Specification specifically for battery production. The goal is to make a single global standard.

6.2 Workflow and Data Exchange

The integration enables the creation of a strategic workflow that synchronises virtual and physical testing environments, maximising the utilisation of testing resources.

- Model Selection and Test Request: When a test request is made, the DT communicates with the LIMS to retrieve the appropriate models and data for the Unit Under Test (UUT) [24]. The LIMS shows the safety and reliability models from the WP4 toolchain as virtual test benches.
- Task Distribution and DoE: The Intelligent Design of Experiments (DoE) algorithm from WP2 determines the optimal approach for testing, such as whether it should be conducted in person or online.
- Virtual Testing and Data Feedback: If you choose a virtual test, the WP4 toolchain models are run. After that, the results are sent back to the DT for storage and to the DoE algorithm for evaluation of the model's maturity. This creates a closed-loop feedback system that enables you to continually refine the model and verify its accuracy against experimental results.
- Integration with LIMS: The LIMS is the central hub that controls how resources are used, when tests are scheduled, and how data is shared between the DT, the virtual test benches (WP4 toolchain), and the physical test benches.

The FASTEST project's goals of accelerating R&D and enhancing battery design rely on this integrated, data-driven workflow.

7. Validation, Verification, and Continuous Improvement

It is essential to ensure that the integrated WP4 toolchain is scientifically sound, industrially robust, and compliant with all relevant regulations. A comprehensive, multi-tiered Validation and Verification (V&V) protocol is executed in alignment with the stipulations of D4.1 and the overarching FASTEST project framework.

7.1 Validation Protocol and Procedures

The toolchain is thoroughly validated at various hierarchical tiers, encompassing individual model components to the complete system-level architecture.

- Scenario-Based Testing: Scenario-based testing is conducted to ensure that the project's three use cases (automotive, stationary, and off-road) are valid. This testing covers a wide range of operational and abuse conditions. These thorough test scenarios ensure that the toolchain can accurately predict how the battery will behave in all expected operating conditions.
- Benchmarking and Cross-Validation: To ensure the accuracy of the toolchain's outputs, they are cross-validated against known reference models and compared to high-resolution experimental datasets. VTT and FLANDERS MAKE, the project's partners, use the latest experimental facilities to do these validation tests. Electrochemical Impedance Spectroscopy (EIS) and other advanced characterisation methods provide valuable information for verifying and adjusting model parameters.
- Standards-Driven Verification: Verification processes adhere to international standards, including IEC 61508 and ISO 26262. This includes testing the model components individually, testing the interfaces and data flows together, and testing the entire system from start to finish in both the DT and hybrid platform environments. These systematic verification protocols make sure that functional safety requirements and regulatory standards are met. They also establish a clear connection between V&V activities and the confirmation measures and verification reviews required for certification.

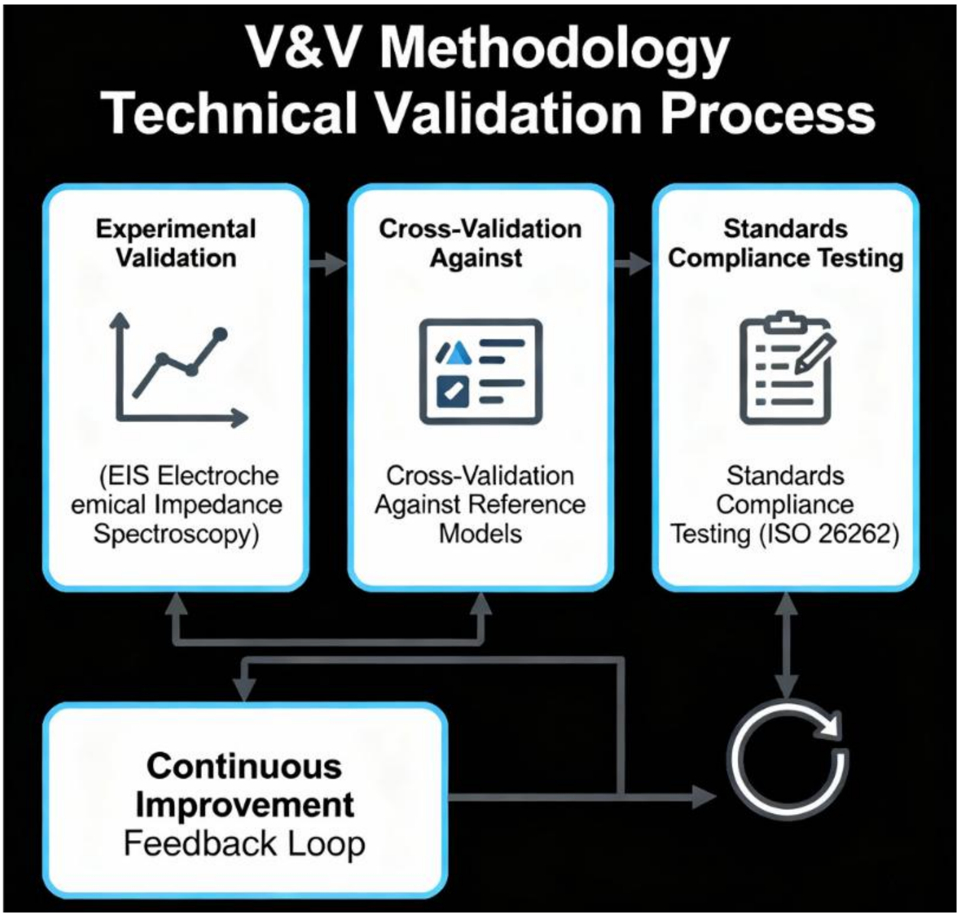

Figure 5 - Validation and Verification Process - Comprehensive V&V Framework

7.2 Feedback Mechanisms for Continuous Improvement

A key part of the toolchain is the incorporation of robust feedback systems that facilitate ongoing improvement. These mechanisms are the operational embodiment of the Digital Twin concept. They transform it from a static model into a living entity that evolves in response to the physical asset's changes.

- Iterative Refinement: The V&V process goes in circles. When there are differences between virtual and physical test results, models are changed and recalibrated. This data-driven feedback loop, which utilises real-world data from the hybrid testing platform (WP6) and the DT (WP5) to refine the virtual models (WP4), ensures that the virtual world remains true to life throughout the battery's entire lifecycle. This ongoing process ensures that the toolchain remains accurate and helpful as new data becomes available and battery technology advances.
- Adaptive AI/ML Algorithms: The feedback systems also let AI/ML algorithms adaptively tune themselves, which improves their performance and ability to generalise over time. Machine learning models improve their predictive capabilities and become more stable when they are continually exposed to new operational data. This method ensures that the virtual models remain effective even when the physical battery wears out or is used in unintended ways. This represents a significant departure from traditional simulation, which is typically a one-time event that occurs during the design phase.

8. Impact and Future Directions

8.1 Impact of the Integrated Toolchain

The creation and use of the high-fidelity, AI-powered multi-domain toolchain in the FASTEST project is a big step forward in how we test battery safety and reliability. The toolchain is expected to have a significant impact, as it will enable extensive virtual testing and predictive diagnostics.

- Accelerated and Cost-Effective Battery R&D: The toolchain helps reduce the time and cost required to develop new battery systems by minimising the need for physical experiments, which are time-consuming and expensive. Early studies indicate that R&D costs could decrease by 34–35% and time could decrease by 41–42%, depending on the specific situation.
- Improved Battery Performance and Safety: The toolchain helps designers create batteries that are more reliable, safer, and last longer by allowing them to examine potential failures and breakdowns more closely during the design phase. This helps reach ambitious performance goals for cars, trucks, and off-road vehicles.
- Enhanced Competitiveness of European Industry: The FASTEST platform and its toolchain will make the European battery industry more competitive across the entire value chain by streamlining the battery development process. This helps the European battery manufacturing industry grow faster, become more innovative, and become more sustainable.

8.2 Future Directions

The toolchain's modular and extensible design makes it easy to add new features and make future changes. As AI and machine learning techniques continue to improve and high-quality data become more widely available, there will be more opportunities to enhance the toolchain's capabilities. Future research will focus on:

- Extension to New Technologies: Adapting the toolchain to work with new battery chemistries (like solid-state, sodium-ion, and lithium-sulfur) and new system architectures.
- Continuous Improvement: Using the ongoing feedback loop between the virtual and physical worlds to make the models even more accurate at making predictions. As machine learning algorithms improve, they will be able to make more accurate predictions and more accurately measure uncertainty.
- Wider Application: Utilising the toolchain in new areas, such as grid-scale energy storage, aerospace, marine applications, and advanced mobility solutions.

9. Conclusion

D4.3, this deliverable, has explained how the AI-powered multi-domain toolchain for battery safety and reliability assessment was successfully integrated and optimised at the system level within the FASTEST project. This work has progressed beyond creating models for individual cells to develop a unified, multi-scale computational environment that enables comprehensive virtual testing and analysis of entire battery modules and packs.

A significant success has been the successful integration of advanced physics-based, data-driven, and AI/ML models into a framework that can be applied in various ways. At the system level, employing critical safety and reliability assessment methods, such as FMEA and hazard analysis, enables the identification of potential design flaws and weaknesses early on. Additionally, strong connections between the Digital Twin (WP5) and the hybrid testing platform (WP6), based on industry standards such as FMI and OPC UA, have enabled seamless collaboration between the virtual and physical testing areas. The primary objective of this project is to expedite the battery R&D cycle and reduce development costs, and this integration plays a significant role in achieving that goal.

The methods and structures outlined in this report offer a robust basis for the concluding phases of validation and verification. The toolchain's extensible design ensures it will be able to keep pace with emerging technologies in the future, benefiting the battery research community and industry stakeholders for a long time after the project concludes. The FASTEST consortium is dedicated to keeping the toolchain up to date with new technologies and industry standards, ensuring it remains useful and continues to have an impact on the future of battery system engineering.

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