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FASTEST

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

Deliverable D4.2: High Fidelity Battery AI-Powered Multi-Domain Toolchain – Safety and Reliability Development.

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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 Digital Twin 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 physics-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
AI	Artificial Intelligence
API	Application Programming Interface
CINEA	European Climate, Infrastructure and Environment Executive Agency
CNN	Convolutional Neural Networks
DoE	Design of Experiments
DT	Digital Twin

FMI	Functional Mock-up Interface
FMU	Functional Mock-up Unit
IEC	International Electrotechnical Commission
ISO	International Organization for Standardization
LIMS	Laboratory Information Management Systems
LSTM	Long Short-Term Memory
ML	Machine Learning
NMC/Si-C	Nickel-Manganese-Cobalt/Silicon-Carbon
OPC UA	Open Platform Communications Unified Architecture
RNN	Recurrent Neural Networks
SAE	Society of Automotive Engineers
SEI	Solid Electrolyte Interphase
SEM	Scanning Electron Microscopy
SRIA	Strategic Research and Innovation Agenda
TEM	Transmission Electron Microscopy
TRL	Technology Readiness Level
V&V	Validation and Verification
WP	Work Package

Table of Contents

1. EXECUTIVE SUMMARY 6
2. INTRODUCTION 7
3. Advanced Multi-Scale Modeling and Integration Framework for Battery System Safety and Reliability 8
4. Safety and Reliability Assessment Methodologies 12
5. Artificial Intelligence and Machine Learning Techniques 15
6. Interfaces and Integration with Digital Twin and Hybrid Testing Platform 17
7. Validation, Verification, and Continuous Improvement 19
8. Interfaces, Interoperability, and Integration 22
9. Impact and Future Directions 24
10. Conclusion 26
11. References 27

List of Figures

Figure 1 - Toolchain Architecture Overview 8
Figure 2 - Multi-Scale Modeling Hierarchy 12
Figure 3 - Safety and Reliability Assessment Workflow 13
Figure 4 - AI/ML Integration Framework 16
Figure 5 - Interoperability approach of FASTEST 18
Figure 6 - Validation and Verification Process 20

1. EXECUTIVE SUMMARY

The FASTEST project aims to significantly speed up and reduce the risk associated with the research and development lifecycle of advanced battery systems by coordinating a complex integration of virtual and physical testing methodologies. Work Package 4 (WP4) plays a crucial role in this ambitious framework, as it is tasked with designing, creating, and implementing a cutting-edge toolchain that enables a thorough virtual assessment of battery safety and reliability. This toolchain is intended as a comprehensive, multi-domain platform that carefully considers the various impacts of ageing, degradation, and a range of abuse scenarios [16]. These factors are becoming increasingly crucial as battery technologies diversify and demand for applications rises.

The current deliverable, D4.2, provides a comprehensive explanation of the technical implementation of this toolchain, detailing its fundamental modelling elements, architectural underpinnings, and sophisticated computational methods used to ensure reliable, accurate, and scalable safety and reliability evaluations. Modern artificial intelligence and machine learning algorithms, data-driven surrogates, and high-fidelity physics-based models can all be seamlessly integrated thanks to the toolchain's naturally extensible and modular architecture. This enables the platform to capture both the stochastic and deterministic aspects of battery failure mechanisms across a broad range of operational contexts, including stationary and off-road applications, as well as automotive chemistries such as NMC/Si-C and solid-state systems.

Additionally, D4.2 describes the methods used to ensure the toolchain is compatible with the larger FASTEST ecosystem, including the hybrid testing platform and the Digital Twin infrastructure. The strict validation and verification procedures used, which utilise both experimental and real-world operational data to calibrate, test, and continuously improve the toolchain's predictive capabilities, receive particular attention. Advanced AI/ML techniques, such as ensemble learning for risk quantification, deep neural networks for anomaly detection, and hybrid physics-informed models for predictive diagnostics, are integrated into the toolchain to enhance virtual testing fidelity and facilitate proactive risk management and decision support throughout the battery system's lifecycle [13].

The technical and methodological developments realised in WP4 are summarised in this deliverable, which shows how integrating state-of-the-art modelling, data analytics, and AI/ML techniques into a single toolchain framework can significantly improve the efficiency, dependability, and safety of developing next-generation battery systems.

2. INTRODUCTION

The multi-domain toolchain, created as part of the FASTEST project's Work Package 4 (WP4), is envisioned as a high-fidelity, modular computational environment painstakingly designed to model and assess the safety and dependability of battery systems at multiple hierarchical levels, from individual electrochemical cells to fully integrated battery packs. Due to its purposeful, chemistry-agnostic design, this toolchain can be applied in a wide range of application domains, including stationary energy storage, off-road electrification scenarios, and automotive propulsion. It supports both Generation 3b (nickel-manganese-cobalt/silicon-carbon, NMC/Si-C) and Generation 4 (solid-state) cell chemistries.

The toolchain's primary goal is to provide a comprehensive virtualised environment for the rigorous evaluation of safety and dependability, significantly reducing the reliance on labour-intensive and resource-intensive physical experimentation. To identify latent failure modes and quantify associated risks before physical prototyping, a paradigm that is gaining increasing support in current battery research and development, the platform utilises sophisticated simulation capabilities to enable the investigation of a broad range of operational and abuse conditions [15].

The toolchain's incorporation of sophisticated ageing and degradation models, which are crucial for risk assessment and predictive diagnostics across the battery lifecycle, is one of its unique features. Drawing on recent developments in both physics-based and data-driven modelling approaches, these models capture capacity fade, impedance growth, calendar and cycle ageing phenomena, and the stochastic nature of degradation processes [4][5]. By utilising these models, the toolchain can predict how vital performance and safety metrics will evolve under various usage patterns, environmental conditions, and abuse scenarios. This helps to support proactive maintenance and risk reduction.

The smooth transfer of data and models, facilitated by the Digital Twin infrastructure (WP5) and the hybrid testing platform (WP6), further ensures interoperability and scalability. To facilitate co-simulation, real-time data synchronisation, and the integration of heterogeneous modelling assets, the toolchain utilises standardised interfaces, such as the Functional Mock-up Interface (FMI) [13]. In addition to improving the platform's adaptability and scalability, this architectural decision supports new best practices in cyber-physical systems engineering and the digitalisation of battery research and development [1][18].

Importantly, the toolchain leverages cutting-edge artificial intelligence and machine learning (AI/ML) methods to enhance the precision, resilience, and computational efficiency of safety and dependability evaluations. The platform can capture complex, nonlinear dependencies and rare-event phenomena that are frequently unmanageable with traditional modelling approaches alone by combining deep learning architectures, ensemble methods, and hybrid physics-informed models [20]. This facilitates the rapid development and implementation of next-generation battery technologies by allowing the toolchain to provide high-fidelity predictions and actionable insights across a wide range of chemistries, architectures, and operational contexts.

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

3.1 A Service-Oriented, Modular Framework

The architecture of the WP4 toolchain is constructed on a service-oriented, modular framework, purpose-built to ensure robust interoperability with a diverse array of external platforms and systems. This design paradigm enables the seamless integration and orchestration of heterogeneous modelling approaches, including reduced-order, data-driven, and high-fidelity physics-based models. Each model is meticulously engineered to analyse specific facets of battery behaviour under both typical and adverse operating conditions.

In practical terms, this modularity allows users to flexibly incorporate new modelling techniques as innovation in battery technology evolves, supporting ongoing validation and refinement of predictive analytics. By leveraging Application Programming Interface (APIs) [NT2] and standard communication protocols, the toolchain can readily exchange data with simulation environments, laboratory management systems, or cloud-based analysis services. For example, reduced-order models might be used for real-time diagnostics within embedded systems, while high-fidelity simulations can inform research on failure mechanisms or optimise cell design. The WP4 toolchain's comprehensive approach supports both industrial deployment and academic research, promoting collaboration across disciplines and enabling rapid adaptation to emerging challenges in battery system development. Sometimes ‚modelling' is used and other times ‚modeling' use the same everywhere.

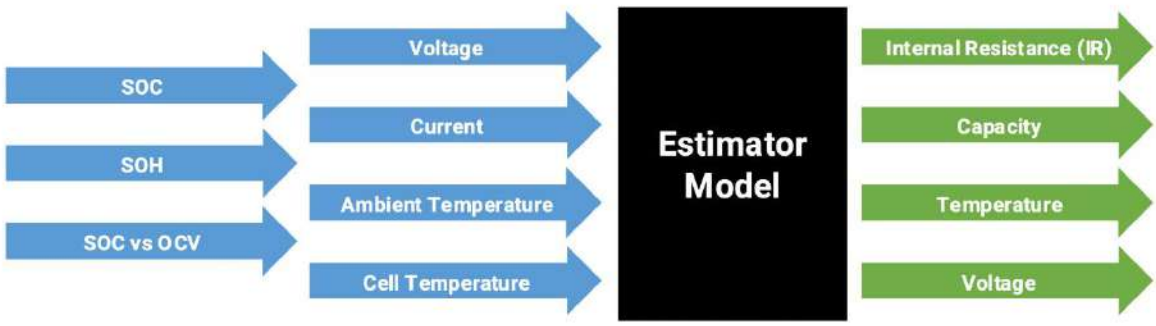

Figure 1 - Toolchain Architecture Overview

3.2 Granular Modeling: Fidelity at the Cell Level

At the most detailed level, the toolchain utilises advanced mechanical, thermal, and electrochemical models to elucidate the fundamental processes governing battery performance, deterioration, and failure at the single-cell level. A high degree of predictive fidelity and scientific credibility is ensured by these models' rigorous parameterisation using high-resolution experimental datasets and systematic validation against empirical test results.

Four common degradation phenomena were implemented first on the single-particle level model in WP3, namely solid electrolyte interphase (SEI) growth, lithium plating, particle cracking, and stress-enhanced diffusion. These mechanisms were chosen as they represent the most probable mechanisms for capacity fade and impedance rise in modern Li-ion cells under a wide range of operating conditions.

The single-particle models provide a mechanistic description of the local electrochemical, transport, and mechanical processes that govern the long-term evolution of the electrodes. The degradation models were systematically coupled with the electrochemical performance model of the whole cell in WP3. This integration enables the coupled study of how particle-scale degradation is reflected in the macroscopic level of voltage response of the single cell.

To facilitate integration into higher-level simulation environments (in this case, the high-fidelity multi-domain toolchain), the coupled electrochemical performance model and ageing models were exported as a Functional Mock-up Unit (FMU), ensuring compatibility with co-simulation workflows and interoperability with other domains. The FMU serves as the central battery performance model within the multi-domain, high-fidelity toolchain developed in the project.

By introducing physically meaningful degradation mechanisms, the extended electrochemical model surpasses traditional capacity fade approximations and enables the simulation of realistic operating conditions, including fast charging and temperature fluctuations. The predictive capability of the model extends not only to standard cycling performance but also to the interplay of local degradation phenomena, which can trigger accelerated failure modes under critical conditions. Furthermore, the toolchain enables users to explore the interplay of localised phenomena—such as lithium plating, electrode cracking, and electrolyte decomposition—that contribute to cell ageing and catastrophic failure events.

The validation of the implemented ageing models can be carried out indirectly by comparing the predicted evolution of battery capacity loss with experimental measurements during cycling. Direct quantification of degradation modes, such as SEI growth or lithium plating, remains challenging because these processes occur at the nanoscale and are not easily measured using post-mortem techniques, including scanning electron microscopy (SEM) or transmission electron microscopy (TEM). Instead, the approach taken relies on correlating the integrated effects of these mechanisms, which manifest as capacity loss, with measured cycling data. By adjusting the model parameters within physically reasonable ranges, the simulated trends of capacity loss can be aligned with the experimental observations. This approach gives confidence that the underlying main degradation phenomena are represented with sufficient fidelity. This indirect validation strategy is consistent with the current state of the art in battery ageing research, where electrochemical models are validated against macroscopic performance indicators rather than direct microscopic evidence.

Furthermore, the integration of real-time sensor data and historical usage patterns into the modelling environment supports dynamic recalibration and continuous improvement of predictive accuracy. This adaptive capability allows for the early detection of deviations from expected behaviour, facilitating both preventive maintenance strategies and the development of safer, longer-lasting battery technologies. By bridging the gap between micro-scale phenomena and practical system-level outcomes, the toolchain establishes a robust foundation for the design, optimisation, and risk assessment of next-generation battery systems.

3.3 Integration at Multiple Scales: Module and Pack-Level Structures

The toolchain integrates cell-level models into larger modules and packs, accounting for inter-cell variability, thermal management, electrical balancing, and complex system interactions. This multi-scale approach enables the simulation of scenarios like local failure propagation and the assessment of overall system resilience, reflecting real-world applications.

By incorporating granular cell-level data, the toolchain ensures that variations in manufacturing quality, cell ageing, and operational conditions are accurately represented across the battery pack. Its advanced algorithms enable sophisticated thermal management modelling, predicting hot spots and facilitating design optimisation to prevent thermal runaway events. Electrical balancing is precisely simulated, ensuring uniform state-of-charge distribution and mitigating risks associated with overcharging or deep discharging individual cells. Furthermore, the toolchain's capability to model complex system interactions—such as the effects of rapid charge/discharge cycles, environmental stressors, and dynamic load demands—allows engineers to visualise and address emergent behaviours at the pack and module level.

With this comprehensive framework, users can run predictive analyses on how faults or failures could propagate through a system, gaining insight into failure modes and enhancing the resilience of the entire architecture. Such simulations are crucial in industries such as electric vehicles, grid storage, and aerospace, where reliability and safety are paramount. By bridging detailed electrochemical behaviour with large-scale system dynamics, the toolchain empowers researchers and engineers to optimise designs, reduce development cycles, and accelerate innovation in energy storage technology.

3.4 Lifecycle Integration and Bidirectional Data Flows

The toolchain supports bidirectional data flows, enabling real-time ingestion of operational data for calibration, validation, and learning. Simulation results can be exported to both Digital Twin infrastructure and hybrid testing platforms. This facilitates scenario analysis, closed-loop co-simulation, and informed decision-making throughout the battery system lifecycle.

Building upon this robust framework, the toolchain empowers engineers and stakeholders to seamlessly integrate live operational feedback into their models, ensuring that calibration and validation processes are not only faster but also more precise. Real-time learning capabilities enable adjustments to be made on the fly, allowing for swift adaptation to new data or unexpected conditions. By exporting simulation outcomes to Digital Twin ecosystems and hybrid testbeds, users gain a comprehensive understanding of system behaviour across both virtual and physical domains. As a result, organisations can conduct detailed scenario analyses, anticipate potential challenges, and optimise performance via closed-loop co-simulation. Ultimately, this approach fosters more reliable, efficient, and intelligent decision-making throughout every phase of the battery system’s development and operation.

3.5 Interfaces Based on Standards and Future-Proof Extensibility

The toolchain's interfaces are developed in accordance with industry standards, including the Functional Mock-up Interface (FMI) specification, to support broad compatibility and potential extensibility. This approach is designed to facilitate integration with various simulation and data management environments and follows commonly adopted practices for digitalising battery research and cyber-physical systems engineering. As a result, the toolchain serves as a flexible and interoperable platform designed to address current and future requirements in advanced battery system development.

By adhering to widely recognised protocols, the toolchain ensures seamless interaction between diverse software and hardware components—a critical feature for multidisciplinary teams engaged in battery innovation. The FMI standard, in particular, allows users to efficiently exchange models and results across different simulation environments without sacrificing fidelity or usability. This collaborative interoperability helps streamline workflows, accelerate design iterations, and reduce overhead caused by incompatible tools.

Furthermore, the toolchain's commitment to extensibility positions it well for evolving research landscapes. As emerging challenges in energy storage and cyber-physical systems arise, the platform can readily incorporate new methodologies, datasets, and analytical techniques to address these challenges. This adaptability not only future-proofs investments but also fosters a sustainable ecosystem for continuous improvement and knowledge sharing among stakeholders.

Ultimately, this robust and forward-looking infrastructure empowers engineers, researchers, and industry partners to push the boundaries of battery technology, driving advancements that meet the demands of next-generation applications, such as electric vehicles, grid storage, and portable electronics.

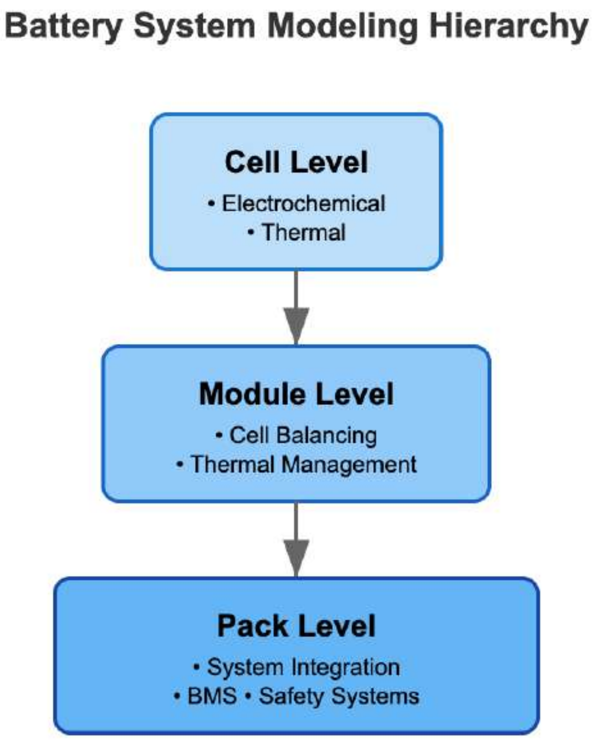

Figure 2 - Multi-Scale Modeling Hierarchy

4. Safety and Reliability Assessment Methodologies

4.1 Integrated Modeling Environment for Failure and Degradation Analysis

The WP4 toolchain's safety and reliability assessment capabilities are underpinned by a comprehensive, multi-layered suite of models and algorithms, enabling the simulation, diagnosis, and evaluation of a broad spectrum of failure modes, degradation mechanisms, and abuse scenarios characteristic of advanced battery systems. This integrated modelling environment is designed to capture the intricate interactions between mechanical, thermal, and electrochemical processes, as well as the stochastic and path-dependent nature of battery ageing and failure phenomena [1][5].

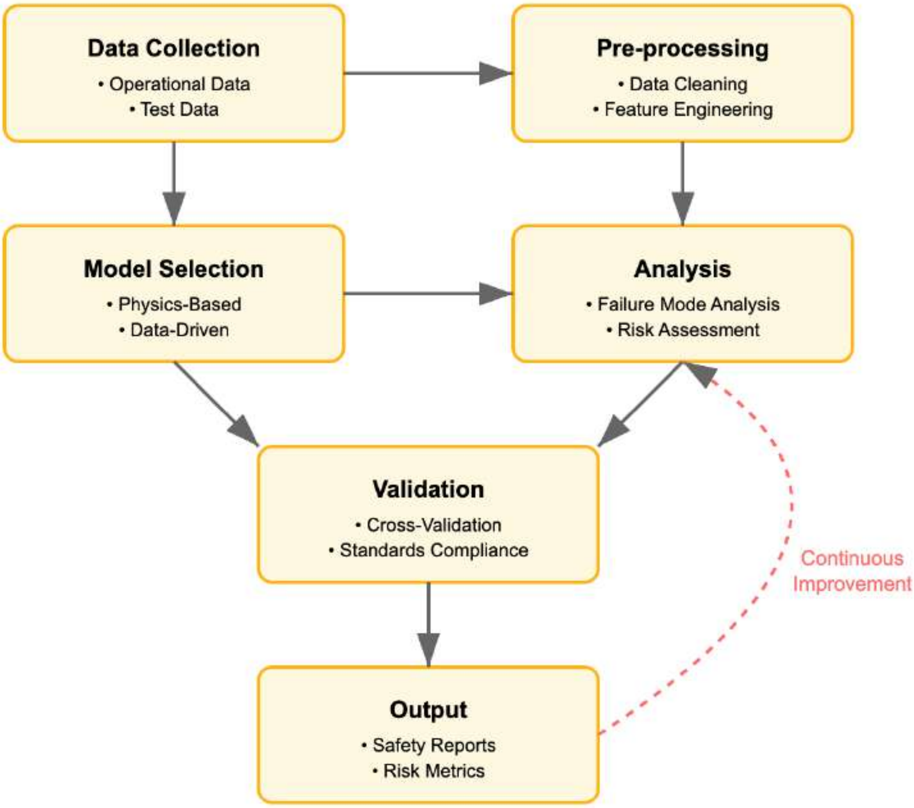

Figure 3 - Safety and Reliability Assessment Workflow

4.2 High-Fidelity Physics-Based Modeling

At the core of the toolchain are high-fidelity, physics-based models that replicate the fundamental mechanisms influencing battery behaviour. These models incorporate detailed representations of electrochemical kinetics, heat generation and dissipation, and mechanical deformation, thereby enabling the prediction of critical events such as thermal runaway, internal short circuits, and structural failure under both normal and abusive operating conditions [7][15]. The onset and propagation of these failure modes are modelled using coupled multi-physics approaches, which have been validated against experimental data and are consistent with the latest advances in battery safety research.

4.3 Advanced Ageing and Degradation Models

Complementing the physics-based models are advanced ageing models that characterise the effects of capacity fade, impedance growth, and both calendar and cycle ageing [4]. These models are parameterised using a combination of field data and laboratory-based experiments, allowing for the accurate prediction of long-term performance degradation and the identification of precursors to catastrophic failure [17]. Their integration within the toolchain supports the development of predictive diagnostics and facilitates the implementation of risk-informed maintenance strategies.

4.4 Data-Driven and Machine Learning Approaches

The toolchain also incorporates data-driven models that leverage machine learning algorithms and historical test data to forecast the probability and outcomes of specific abuse scenarios, such as overcharge, overdischarge, and exposure to extreme temperatures [18]. These models are trained on large datasets encompassing a wide range of operational and failure events, enabling the detection of subtle patterns and correlations that may elude traditional modelling techniques [14]. The adoption of data-driven approaches enhances the toolchain's generalisability across different chemistries, architectures, and use cases, and supports the continuous improvement of safety and reliability assessments as new data becomes available.

4.5 System-Level Aggregated Modeling

Based on the previously described granular, high-fidelity cell models, the toolchain uses aggregated models to assess safety and reliability at both module and pack levels. The toolchain can precisely account for complex system interactions, electrical protection, thermal control, and cell balancing by incorporating these intricate cell-level representations into a comprehensive system context.

Designing robust battery systems requires the ability to simulate both steady-state and transient conditions. This integrated approach enables the tracking of failure propagation and the evaluation of the system's overall resilience. The toolchain provides engineers with practical insights into potential weaknesses and performance issues in battery architectures by utilising these thorough modelling techniques. Before physical prototyping, teams can proactively address design flaws thanks to its sophisticated simulation capabilities, which support predictive analytics. By enabling quick virtual testing of design changes under various operating conditions, the toolchain also promotes iterative optimisation, which lowers development costs and time. Stakeholders can enhance overall system robustness, longevity, and regulatory compliance in demanding real-world applications, such as grid energy storage and electric vehicles, by utilising comprehensive visualisation and reporting tools to inform their decisions.

4.6 Standards Compliance and Best Practices

The toolchain is designed to comply fully with relevant international standards for battery safety and reliability testing, such as SAE J2464 and ISO 26262. This compliance ensures that virtual safety and reliability assessments performed within the toolchain adhere to industry best practices, facilitating the systematic identification of critical failure modes, quantitative risk evaluation, and the implementation of robust mitigation strategies. By offering a comprehensive and adaptable platform for safety and reliability analysis, the WP4 toolchain accelerates the development and deployment of advanced battery technologies while upholding the highest standards of safety and reliability in operation.

Furthermore, the WP4 toolchain integrates a suite of analytical modules tailored for diverse battery architectures and operating conditions, enabling both manufacturers and researchers to efficiently simulate real-world scenarios. This allows stakeholders to predict performance outcomes, anticipate potential hazards, and make informed design decisions early in the product development lifecycle. The user-friendly interface ensures seamless adoption by cross-functional teams, promoting collaboration between engineers, safety specialists, and regulatory bodies.

By supporting traceable documentation and automated reporting that aligns with regulatory requirements, the toolchain streamlines the certification process and reduces the time-to-market for new products. Its scalability ensures it remains effective for emerging battery chemistries and evolving industry requirements, making it a vital asset for organisations seeking to achieve operational excellence and maintain a competitive edge in the rapidly changing field of battery technology. Ultimately, the WP4 toolchain empowers users to deliver safer, more reliable battery systems that meet rigorous global standards and expectations.

5. Artificial Intelligence and Machine Learning Techniques

5.1 Strategic Integration of AI/ML in Battery Assessment

The systematic integration of advanced artificial intelligence (AI) and machine learning (ML) methodologies is a defining innovation of the WP4 toolchain, fundamentally enhancing the operational efficacy, resilience, and predictive power of safety and reliability evaluations for complex battery systems. By leveraging these approaches, the toolchain transcends the limitations of traditional deterministic modelling, enabling the extraction of actionable insights from high-dimensional, heterogeneous datasets and supporting proactive risk management across a broad spectrum of operational scenarios [14][18].

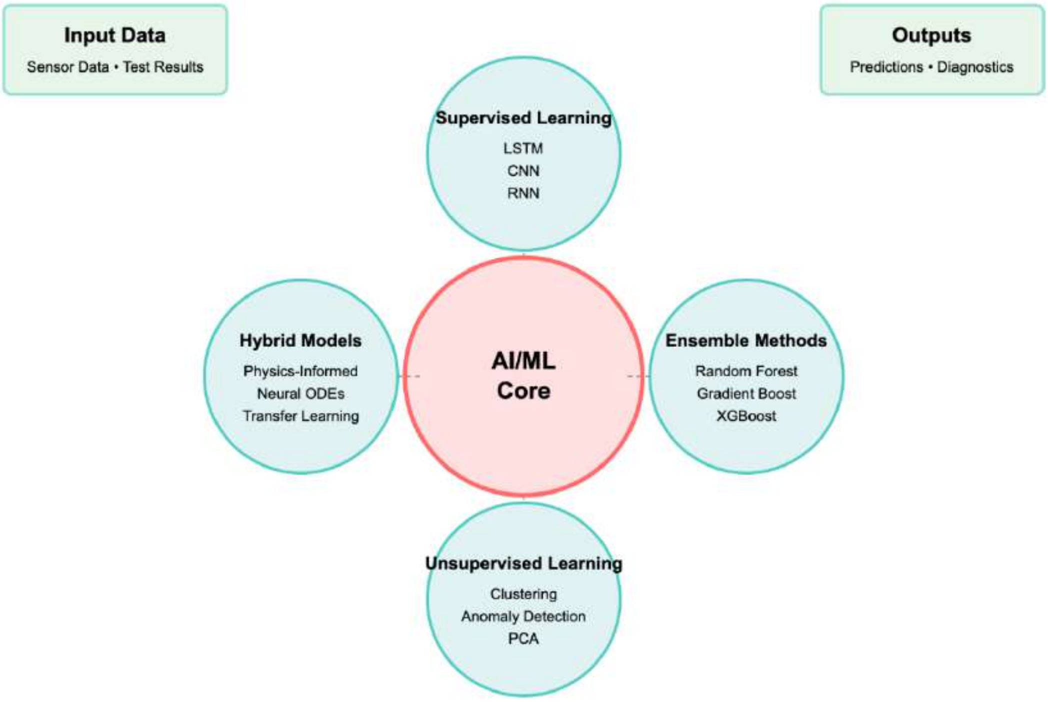

Figure 4 - AI/ML Integration Framework

5.2 Supervised Learning for Predictive Diagnostics

Central to this strategy is the deployment of supervised learning algorithms, including long short-term memory (LSTM) architectures, recurrent neural networks (RNNs), and convolutional neural networks (CNNs) [10]. These models are adept at analysing time-series data derived from both simulated environments and empirical testing, detecting subtle temporal patterns and signatures indicative of impending failure, abnormal degradation trajectories, or hazardous operational states [22]. Trained on extensive datasets encompassing both nominal and abusive conditions, these models endow the toolchain with robust early warning and predictive maintenance capabilities, facilitating real-time anomaly detection and the anticipation of critical events before they escalate to system-level failures.

5.3 Ensemble and Decision Tree-Based Methods for Risk Analysis

For risk assessment, fault classification, and root cause analysis, the toolchain utilises decision tree-based algorithms and ensemble learning methods, including random forests and gradient boosting machines [21]. These models are trained on labelled datasets that capture the full diversity of operational and failure scenarios, enabling the accurate identification, prioritisation, and attribution of critical failure modes. The inherent interpretability of these models supports transparent decision-making and the development of targeted mitigation strategies, which are essential for both regulatory compliance and operational safety [20].

5.4 Unsupervised Learning for Emerging Risk Detection

The toolchain also incorporates unsupervised learning techniques, including anomaly detection frameworks and clustering algorithms, to interrogate large-scale operational datasets for rare or previously unobserved failure patterns [11]. This capability is particularly valuable for the continuous evolution of safety and reliability models, as it enables the identification of emergent risks and the dynamic adaptation of assessment methodologies in response to shifting operational landscapes. By embedding these unsupervised methods, the toolchain remains adaptable to new threats and maintains its relevance in rapidly evolving application domains.

5.5 Hybrid Modeling: Bridging Data-Driven and Physics-Based Approaches

A further advancement is realised through the development of hybrid modeling techniques, which synergistically combine the flexibility and data-driven insights of AI/ML algorithms with the interpretability and physical fidelity of mechanistic models [3]. By integrating machine learning components with physics-based and reduced-order models, the toolchain achieves robust generalisation and high predictive accuracy across a wide range of battery chemistries, architectures, and use cases [6]. This hybrid paradigm not only enhances the reliability of virtual testing but also supports the transferability of models to novel systems and operational contexts, thereby future proofing the toolchain against technological advances and evolving industry requirements.

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

6.1 Standards-Based Interoperability and Digital Twin Compatibility

A cornerstone of the WP4 toolchain's operational versatility is its complete compatibility with the Digital Twin architecture developed in Work Package 5 (WP5). This compatibility is realised through the implementation of robust, standards-based interfaces that enable model co-simulation, real-time data exchange, and comprehensive virtual validation of battery systems throughout their lifecycle. By leveraging the Digital Twin paradigm, the toolchain facilitates predictive diagnostics, dynamic scenario analysis, and closed-loop optimisation of battery safety and performance [2][19].

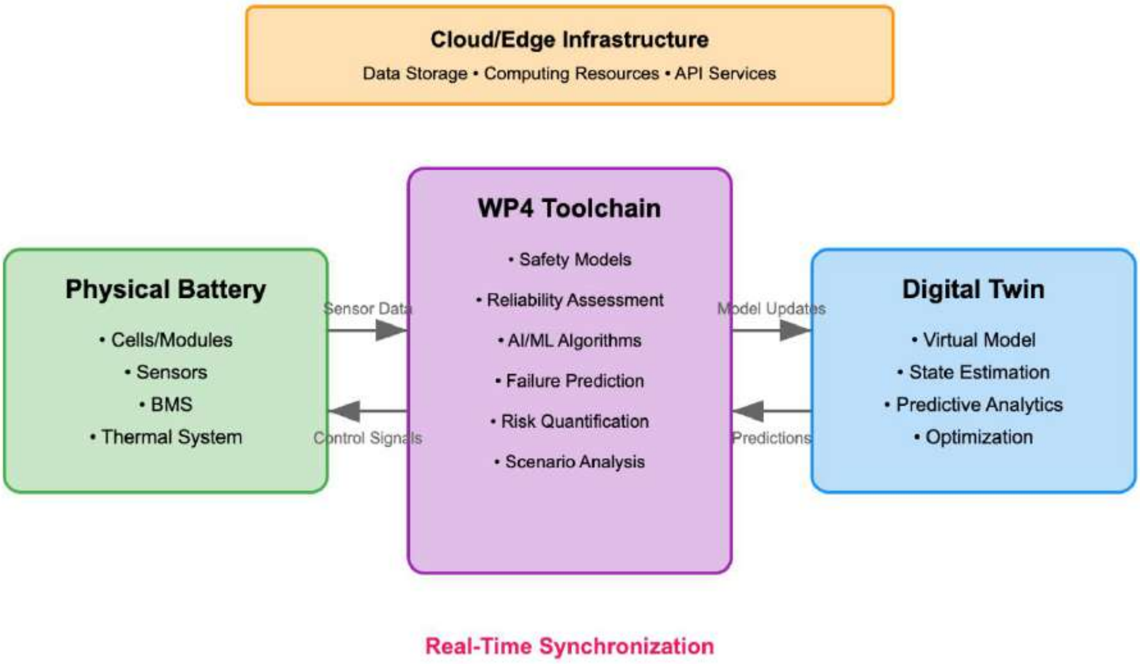

Figure 5 - Interoperability approach of FASTEST

6.2 Protocols and Communication with Hybrid Testing and LIMS Environments

The integration architecture is underpinned by the adoption of standardised data formats and communication protocols, such as the Open Platform Communications Unified Architecture (OPC UA) and the Functional Mock-up Interface (FMI), both of which are widely recognised in the domains of industrial automation and cyber-physical systems [12]. These protocols ensure seamless interoperability not only with the Digital Twin infrastructure but also with the hybrid testing platform and laboratory information management systems (LIMS) specified in Work Package 6. As a result, the toolchain is capable of exporting simulation results, ingesting real-time operational data, and engaging in co-simulation workflows with a diverse array of data sources and modelling assets.

6.3 Strategic Benefits of Standards-Driven Integration

This standards-driven approach to integration confers several strategic advantages. It enables the toolchain to serve as a foundational component within a broader digital ecosystem, facilitating multi-site validation, collaborative development, and the rapid deployment of new models and algorithms [6]. Furthermore, it streamlines regulatory compliance and accelerates the translation of research innovations into industrial practice, aligning with the latest best practices in the digitalisation of battery research and development [20].

6.4 Enabling Next-Generation Battery System Engineering

By providing stable, scalable integration with the Digital Twin and related platforms, the WP4 toolchain is essential to the FASTEST project's next-generation battery system engineering goals. This supports both the technical and broader aims of creating an adaptable and industry-focused digital infrastructure for advanced battery development.

Building on its robust architecture, the WP4 toolchain not only facilitates seamless connectivity across digital platforms but also enhances data accuracy and real-time analytics, which are crucial for informed decision-making throughout the battery lifecycle. Its modular design enables rapid adaptation to evolving engineering requirements, significantly reducing development time and fostering innovation. By embracing cutting-edge digital twin methodologies, WP4 positions the FASTEST project at the forefront of industry trends, enabling stakeholders to anticipate market needs, improve sustainability, and accelerate the commercialisation of breakthrough battery technologies. Ultimately, this collaborative approach ensures that the project delivers impactful solutions that are aligned with both current and future challenges in the energy storage sector.

7. Validation, Verification, and Continuous Improvement

7.1 Multi-Tiered Validation Protocol

Validation and verification (V&V) are foundational to ensuring the scientific reliability, industrial robustness, and regulatory compliance of the WP4 toolchain across a broad spectrum of research and operational contexts. The toolchain is subjected to a comprehensive, multi-tiered validation protocol, which encompasses scenario-based testing under a wide range of operational and abuse conditions, cross-validation with established reference models, and benchmarking against high-resolution experimental datasets [4][5]. This rigorous approach is implemented at multiple hierarchical levels, beginning with the characterisation of individual cells and modules and extending to the assessment of complete packs and system-level architectures. The validation methodology is meticulously aligned with the requirements and procedures articulated in D4.1 and the overarching FASTEST project framework.

7.2 Standards-Driven Verification Procedures

Verification procedures are systematically implemented in accordance with internationally recognised standards, such as ISO 26262 (Road Vehicles – Functional Safety) and IEC 61508 (Functional Safety of Electrical/Electronic/Programmable Electronic Safety-related Systems), to ensure that the toolchain meets all functional and performance specifications as outlined in the project's technical documentation [8][9]. These procedures include unit testing of discrete model components, integration testing of the assembled toolchain, and system-level testing within the Digital Twin and hybrid testing platform environments. The adoption of such standards-driven verification practices guarantees that the toolchain is suitable for deployment in both research settings and safety-critical industrial applications.

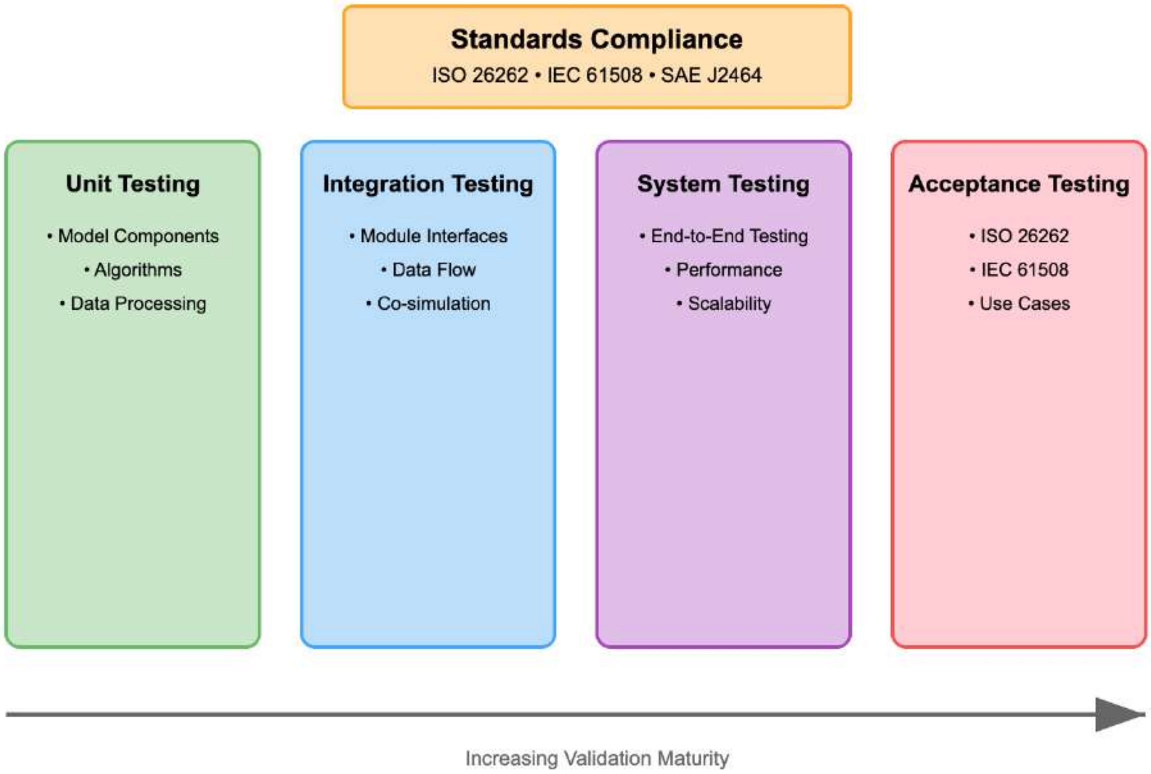

Figure 6 - Validation and Verification Process

The validation/verification of the ageing models is performed through an indirect approach that links experimental data with model predictions. First, experimental cycling data, such as capacity loss, serve as a reference. The electrochemical model with the ageing mechanisms is then coupled with the optimisation algorithm, which tries to minimise the difference (root mean square deviation) between the simulation results and experimental measurements. During this process, the optimisation algorithm adjusts the model parameters until the simulated behaviour matches the measured trends with acceptable accuracy. The result of this methodology is a set of optimised parameters. With the additional measurements performed under different conditions, such as varying temperatures or current rates, the parameter set can be further refined to capture the dependencies of degradation processes on operating conditions.

7.3 Feedback Mechanisms and Iterative Improvement

A critical enabler of continuous improvement is the integration of robust feedback mechanisms within the toolchain architecture. These mechanisms facilitate the adaptive tuning of AI/ML algorithms, the iterative refinement of model parameters, and the dynamic incorporation of new experimental and operational data in response to evolving operational profiles and the emergence of novel failure modes [3][18]. This iterative, data-driven approach ensures that the toolchain maintains its predictive accuracy and operational relevance as battery technologies and application requirements evolve.

7.4 Sustained Value and Future Readiness

Incorporating rigorous verification and validation (V&V) processes and continuous learning, the WP4 toolchain provides an advanced platform for assessing battery safety and reliability. This ensures ongoing value for the FASTEST project and establishes a strong basis for future innovations in battery system engineering.

Building upon a foundation of thorough Validation and Verification (V&V) methodologies, the WP4 toolchain is designed not only to assess battery system performance rigorously but also to adapt and improve through integrated continuous learning capabilities. These features enable the platform to integrate new data, refine existing models, and respond promptly to emerging safety and reliability challenges within the battery domain. By delivering detailed analyses, predictive insights, and actionable recommendations, the WP4 toolchain enables engineers and stakeholders to make informed decisions throughout the development lifecycle. Its robust framework thereby allows the FASTEST to project to achieve both immediate objectives and sustainable progress, positioning the initiative at the forefront of advancements in battery system engineering.

8. Interfaces, Interoperability, and Integration

8.1 Architectural Principles and Digital Ecosystem Compatibility

A foundational design principle of the WP4 toolchain is its robust interoperability with external systems and digital platforms, ensuring seamless integration within the broader FASTEST project ecosystem. The toolchain's architecture is fully compatible with the Digital Twin infrastructure developed in Work Package 5 (WP5), enabling real-time, bidirectional data exchange, model co-simulation, and comprehensive virtual validation of battery systems across their operational lifecycle [2][19]. This compatibility is achieved through the adoption of standardised interfaces and communication protocols, such as the Functional Mock-up Interface (FMI), which facilitate integration with the hybrid testing platform and laboratory information management systems (LIMS) specified in WP6 [12][13].

8.2 Strategic Integration for Resource Optimisation and Adaptive Testing

This integration is not merely technical but strategic, supporting the effective allocation of testing resources, the optimisation of test campaigns, and the continuous synchronisation of virtual and physical testing environments. The toolchain's ability to dynamically orchestrate simulation and experimental workflows empowers stakeholders to conduct scenario-based analyses, accelerate design iterations, and implement adaptive testing strategies that respond to evolving project requirements and operational insights [6]. Such orchestration is essential for maximising the efficiency and agility of battery R&D processes.

8.3 Modularity, Extensibility, and Future-Proofing

The extensibility and adaptability of the toolchain are further enhanced by its modular architecture. This design enables the rapid addition, replacement, or reconfiguration of model components, allowing for swift adaptation to new battery chemistries, system architectures, and emerging use cases. The modularity of the toolchain ensures that it can accommodate regulatory changes and technological advancements without necessitating a complete redesign, thereby future-proofing the platform and supporting long-term sustainability [20].

8.4 Dual-Mode Operation and Lifecycle Value

The toolchain supports both batch and real-time modes, making it suitable for all stages of battery research and development—from simulations and prototyping to field monitoring and predictive maintenance. Its versatility ensures value for academic and industrial users throughout the battery system lifecycle.

In addition to accommodating a wide range of workflows, the toolchain seamlessly integrates with existing data analysis platforms and laboratory hardware, streamlining the transition between experimental phases and large-scale deployment. Advanced analytics and visualisation capabilities enable researchers to rapidly identify trends and anomalies, while robust security protocols safeguard sensitive intellectual property. As a result, both academic institutions and industry partners benefit from accelerated innovation cycles, reduced risk, and improved decision-making at every step of battery technology advancement.

8.5 Enabling Integrated, Data-Driven Battery System Engineering

By incorporating principles of interoperability, modularity, and operational flexibility, the WP4 toolchain contributes to the FASTEST project's goals of developing an integrated, data-driven, and adaptive battery system engineering approach. This approach aligns with the project's technical objectives and provides a digital infrastructure that is scalable and extensible for future development of battery technology.

The FASTEST project is dedicated to advancing next-generation battery systems through innovative engineering processes and state-of-the-art digital solutions. The WP4 toolchain plays a pivotal role within this initiative by enabling seamless integration between different tools, facilitating collaboration across multidisciplinary teams, and allowing for efficient adaptation to evolving technological requirements. Its design ensures that new components or methodologies can be incorporated without disrupting existing workflows, fostering agility and sustained innovation.

Furthermore, by supporting comprehensive data management and real-time analysis, the WP4 toolchain empowers researchers and engineers to make informed decisions throughout the development life cycle. This not only accelerates the pace of discovery and deployment but also strengthens the overall reliability and performance of emerging battery technologies. As the field continues to evolve, the WP4 toolchain's robust and adaptable framework positions the FASTEST project at the forefront of battery system engineering, ensuring long-term relevance and impact.

9. Impact and Future Directions

9.1 Transformative Advances in Battery Safety and Reliability Assessment

The development of the high-fidelity, AI-powered multi-domain toolchain within the FASTEST project marks a significant breakthrough in the field of battery safety and reliability evaluation. By enabling extensive virtual testing, predictive diagnostics, and quantitative risk assessment across a broad spectrum of battery chemistries and application domains, the toolchain delivers substantial reductions in development time and cost, while simultaneously enhancing the safety, dependability, and operational performance of next-generation battery systems [5][18]. This paradigm shift supports a more agile, data-driven approach to battery research and development (R&D), facilitating the rapid identification and mitigation of safety-critical issues.

9.2 Integration and Value Delivery Across the Battery Lifecycle

A major differentiator of the toolchain is its seamless integration with digital twin and hybrid testing platform environments. This integration ensures consistent value delivery throughout the lifecycle of the FASTEST project and beyond, bridging the gap between research, development, and industrial implementation. The toolchain supports rapid prototyping, iterative validation, and the accelerated deployment of innovative battery technologies, thereby enabling a continuous feedback loop between virtual and physical domains [2][19]. Its modular and extensible architecture provides a robust foundation for future enhancements, including the incorporation of novel modelling techniques, the assimilation of additional data sources, and expansion into emerging application areas such as distributed energy systems, advanced mobility solutions, and grid-scale energy storage [6].

9.3 Futureproofing Through AI, Data, and Standards

Looking forward, the ongoing evolution of AI and machine learning methodologies, coupled with the increasing availability of high-quality operational and experimental data, will unlock new opportunities for enhancing and expanding the toolchain's capabilities. The continuous development of industry standards and best practices—such as IEC 62933, ISO 26262, and the Batteries Europe Strategic Research and Innovation Agenda- will further inform and guide the toolchain's evolution, ensuring its continued relevance and impact in a rapidly changing technological landscape [6]. This alignment with evolving standards guarantees that the toolchain remains suitable for both regulatory compliance and industrial deployment.

9.4 Commitment to Innovation and Sustainability

The FASTEST consortium is committed to innovation by continuously aligning its toolchain with emerging technological advancements. By fostering robust collaborations among leading experts in artificial intelligence, digitalisation, and battery science, the consortium ensures that its solutions remain at the cutting edge of battery technology. Through regular reviews and upgrades informed by the latest research and industry trends, the group seeks not only to enhance the performance and safety of battery systems but also to address sustainability concerns, such as reducing environmental impact and improving energy efficiency.

The FASTEST consortium works to keep the toolchain aligned with current technological developments. Through ongoing improvement and the adoption of advances in AI, digitalisation, and battery science, the consortium aims to support the development of safer, more reliable, and environmentally sustainable battery technologies. This approach seeks to maintain the toolchain's relevance for both the research community and industry stakeholders, thereby contributing to progress in battery system engineering.

By providing state-of-the-art resources and fostering knowledge exchange between academia and industry, the consortium helps accelerate the integration of breakthrough innovations into real-world applications. Ultimately, FASTEST is dedicated to shaping the future of battery system engineering, ensuring that stakeholders across the value chain benefit from safer, more efficient, and sustainable energy storage solutions.

10. Conclusion

To summarise, Deliverable D4.2 details the successful implementation and deployment of a high-fidelity, AI-powered multi-domain toolchain for battery safety and reliability assessment within the FASTEST project. This toolchain, contained within a modular and interoperable framework, is the result of the convergence of sophisticated physics-based, data-driven, and AI/ML modelling paradigms. This kind of architecture supports both basic research and large-scale applications by enabling thorough virtual testing and predictive diagnostics across the whole hierarchy of battery systems, from individual cells to entire packs [5][18].

The toolchain's successful integration into the larger FASTEST ecosystem is guaranteed by its smooth compatibility with the Digital Twin and hybrid testing platform environments [2]. The project's strategic goals of enhancing the safety, dependability, and performance standards of next-generation battery technologies, reducing development costs, and accelerating the battery R&D cycle are all made possible by this integration. By best practices in model-based systems engineering and digitalisation, the approaches, models, and interface specifications described in this deliverable provide a strong basis for continuing validation, verification, and continuous improvement [6][19].

Furthermore, the toolchain's modular and extensible design ensures that it will be able to adapt to future technological developments, including the addition of new modelling techniques, the integration of new data streams, and the expansion into new fields like advanced mobility solutions and grid-scale energy storage. The FASTEST consortium's dedication to rigorous validation and ongoing innovation guarantees that the toolchain will continue to be a vital resource for industry stakeholders and the battery research community, providing long-term value and impact both during and after the project's lifecycle.

11. References

[1] - Berecibar, M., Gandiaga, I., Villarreal, I., Omar, N., Van Mierlo, J., & Van den Bossche, P. (2016). Critical review of state of health estimation methods of Li-ion batteries for real applications. Renewable and Sustainable Energy Reviews, 56, 572-587.

[2] - Boschert, S., & Rosen, R. (2016). Digital Twin—The Simulation Aspect. In Mechatronic Futures (pp. 59-74). Springer.

[3] - Chen, C., Zhang, Y., & Wang, Y. (2022). Physics-informed machine learning for battery health management: Methods and applications. Energy AI, 10, 100183.

[4] - Dubarry, M., Baure, G., & Devie, A. (2017). Durability and reliability of EV batteries under electric utility grid operations: Path dependence of battery degradation. Journal of Power Sources, 358, 39-49.

[5] - Edge, J. S., O'Kane, S., Prosser, R., Kirkaldy, N. D., Patel, A. N., Hales, A., ... & Offer, G. J. (2021). Lithium ion battery degradation: what you need to know. Physical Chemistry Chemical Physics, 23(14), 8200-8221.

[6] - European Commission. (2020). Batteries Europe: Strategic Research and Innovation Agenda (SRIA).

[7] - Finegan, D. P., Scheel, M., Robinson, J. B., Tjaden, B., Hunt, I., Mason, T. J., ... & Shearing, P. R. (2015). In-operando high-speed tomography of lithium-ion batteries during thermal runaway. Nature Communications, 6, 6924.

[8] - International Electrotechnical Commission. (2010). IEC 61508: Functional safety of electrical/electronic/programmable electronic safety-related systems.

[9] - International Organization for Standardization. (2018). ISO 26262: Road vehicles -- Functional safety.

[10] - Li, W., Zhang, Y., & Wang, Y. (2021). Remaining useful life prediction of lithium-ion batteries based on a hybrid CNN-LSTM model. IEEE Access, 9, 20741-20752.

[11] - Liu, K., Li, K., Peng, Q., & Zhang, C. (2020). A brief review on key technologies in the battery management system of electric vehicles. Frontiers in Mechanical Engineering, 6, 2.

[12] - Mahnke, W., Leitner, S. H., & Damm, M. (2009). OPC Unified Architecture. Springer.

[13] - Modelica Association Project. (2022). Functional Mock-up Interface (FMI) Standard. https://fmi-standard.org/

[14] - Richardson, R. R., Osborne, M. A., & Howey, D. A. (2017). Gaussian process regression for forecasting battery state of health. Journal of Power Sources, 357, 209-219.

[15] - Safari, M., & Delacourt, C. (2011). Modeling of a commercial graphite/LiFePO4 cell. Journal of The Electrochemical Society, 158(12), A1436-A1447.

[16] - Schmidt, J. P., Karden, E., & Sauer, D. U. (2017). Development of a multi-domain battery model for the simulation of dynamic battery behavior in electric vehicles. Journal of Power Sources, 360, 136-149.

[17] - Schuster, S. F., Brand, M. J., Berg, P., Gleissenberger, M., & Jossen, A. (2015). Lithium-ion cell-to-cell variation and its influence on battery pack performance. Journal of The Electrochemical Society, 162(7), A1036-A1055.

[18] - Severson, K. A., Attia, P. M., Jin, N., Perkins, N., Jiang, B., Yang, Z., ... & Braatz, R. D. (2019). Data-driven prediction of battery cycle life before capacity degradation. Nature Energy, 4(5), 383-391.

[19] - Tao, F., Zhang, H., Liu, A., & Nee, A. Y. C. (2019). Digital twin in industry: State-of-the-art. IEEE Transactions on Industrial Informatics, 15(4), 2405-2415.

[20] - Wang, Z., Chen, L., & Zhang, X. (2020). Digital twin for battery management systems: Key issues and future perspectives. Energy Reports, 6, 272-287.

[21] - Xiong, R., Li, L., Tian, J., & Shen, W. (2018). A data-driven fault diagnosis method for lithium-ion batteries using random forests and decision trees. Journal of Power Sources, 393, 17-24.

[22] - Zhang, Y., Wang, Y., & Li, W. (2020). Early detection of battery faults using deep learning and time-series sensor data. Applied Energy, 279, 115872.