ACCELERATING BATTERY CELL DEVELOPMENT

How product-process linkage, digital end-to-end toolchains and simulation models shorten time to market

Capgemini

PEM | RWTH AACHEN UNIVERSITY

“Consistent digitalization can significantly accelerate development processes and is therefore a crucial factor for the competitiveness of cell manufacturers.”

- Marcus Fiege, Capgemini

CONTENT

1. INTRODUCTION

Interest in electric mobility is continuously increasing, largely due to the growing awareness of sustainability, established CO_2 reduction targets, and the ongoing electrification in the transportation sector. Due to increasing demand, particularly from the electric vehicle sector, lithium-ion batteries are in high demand. Additionally, alternative cell chemistries like sodium-ion batteries are gaining traction due to improved raw material availability and potential cost benefits.

Figure 1 shows the expected global demand and announced capacities for lithium-ion and sodium-ion batteries by region according to the Battery Monitor 2023. It is forecasted that by the year 2030 the global demand will comprise 4,917 GWh. In comparison, the total announced capacity including announcements without a specific timeline amounts to 10,959 GWh. However, it is crucial to approach these numbers with caution, as many of the capacity expansions have only been verbally announced, with concrete plans yet to be established. Particularly, China takes a leading role as the primary exporter of battery technologies, while North America, through initiatives such as the Inflation Reduction Act (IRA), as well as Europe, are striving to catch up.[1]

As a result in Europe, numerous gigafactories currently are either in planning stage or being constructed. Efficiency is a key factor for success and the combination of product and process risks often postpones start of production (SOP) dates. Throughout the development process, there are various challenges and opportunities that can potentially shorten the time to market of battery cells.

The following publication will initially outline these challenges and opportunities. In a second step, a potential solution through an improved development approach for battery cells is presented. The publication is a collaborative work within the “Technology Cluster Battery Cell”.

TECHNOLOGY CLUSTER BATTERY CELL

The “Technology Cluster Battery Cell” is a cooperation of Capgemini, the Chair of Production Engineering of E-Mobility Components (PEM), PEM Motion GmbH and the Fraunhofer Research Institution for Battery Cell Production (FFB). The goal is to bring together research institutions and industrial players to catalyze Ecosystem Innovation, generating new methods and toolchains to accelerate the end-to-end process of battery cell development through to scaled battery production.

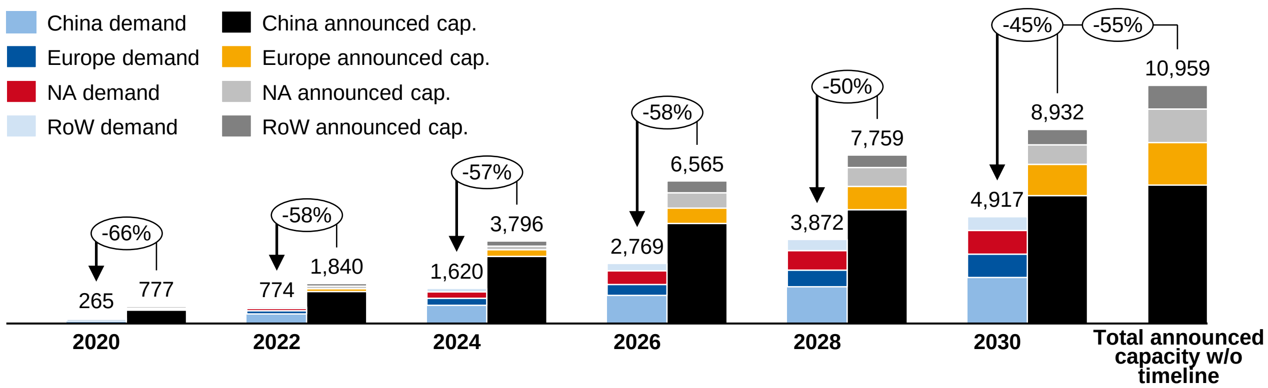
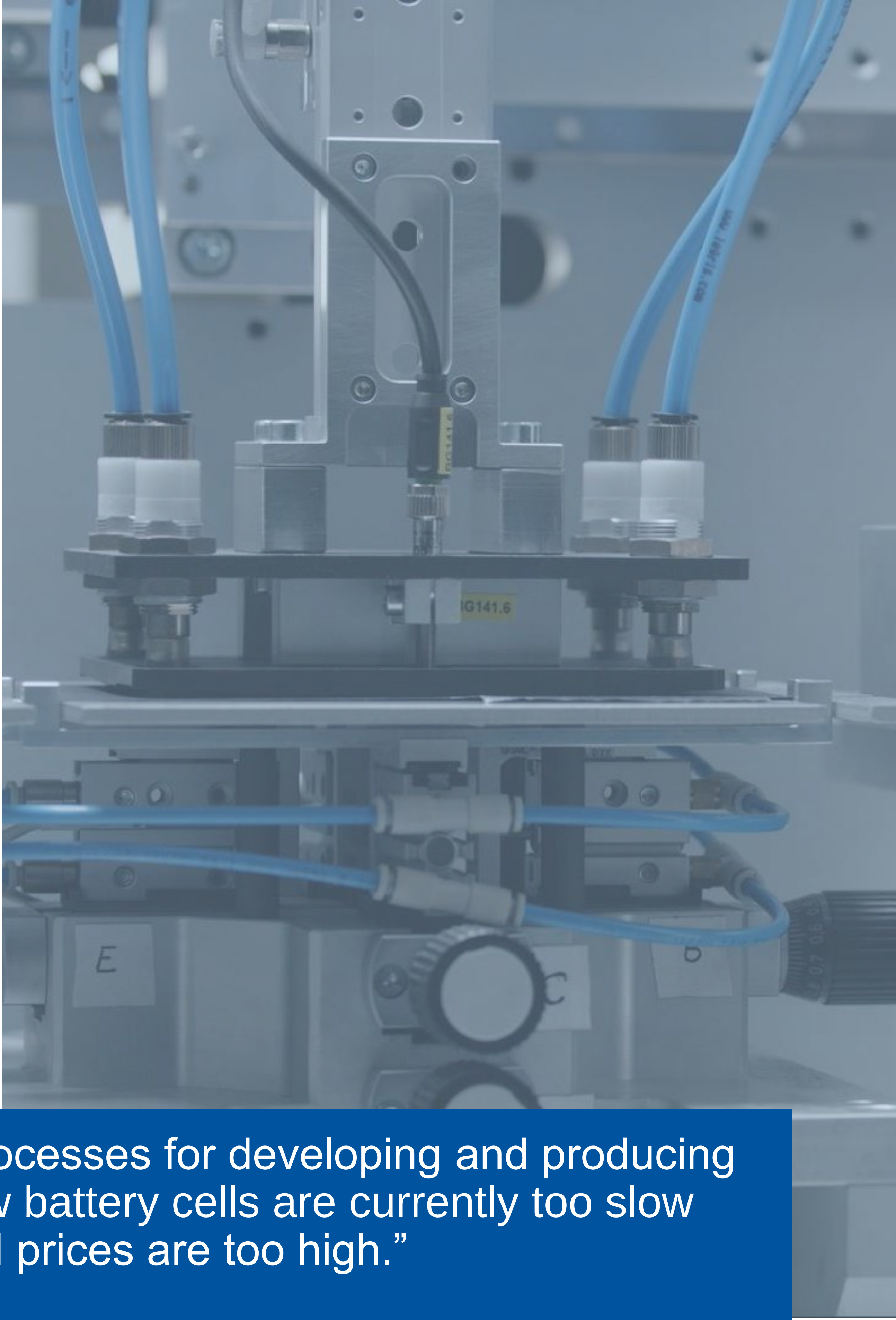


Figure 1: Announced global capacity vs expected demand by region for Li-ion and Na-ion batteries [GWh][1]



“Processes for developing and producing new battery cells are currently too slow and prices are too high.”

- Prof. Achim Kampker, PEM | RWTH Aachen University

2. CHALLENGES AND POTENTIALS OF BATTERY CELL ENGINEERING

To analyze the development process, it is crucial to first examine the current state of the art in the development process of a battery cell, as well as to identify the key challenges and potential opportunities.

The number of available publications stating the development times or ideal development roadmap is limited. The development time of lithium-ion batteries is estimated up to 10 years based on articles and expert knowledge. As an example, the development time is clustered in research and development (5+ years), pre-A-Sample (1-3 years), A-, B-, and C/D-Sample (1-2 years each).[2] Often these phases also overlap. In addition to that reference, the cell development process can also be estimated to take up to 4-6 years based on the authors' industry experience. Figure 2 summarizes a standard development process in the industry based on literature timelines in addition to PEM expertise.

2.1 CHALLENGES OF BATTERY DEVELOPMENT

During the engineering process of lithium-ion batteries, one is confronted with many challenges. The high complexity of both the product and the production process results in lengthy lead times in development, production planning, and ramp-up phase. There is a scarcity of publicly available data and standardized procedures which leads to a lack of transparency in the process chain.

Furthermore, unclear interfaces between development, production, and other departments within a company lead to disjointed processes. Departments may develop and plan without considering others' requirements, causing inefficiencies and a competitive disadvantage, particularly in fast-paced industries like the battery industry, where rapid innovation is a crucial competitive advantage.

2.2 POTENTIALS OF BATTERY DEVELOPMENT

There are also several potentials to address these challenges. Savings in development time and costs can be realized, for instance, through targeted production planning and the shortening or simplification of the ramp-up process. It is important to have an early interface between development and production planning. Additionally, reducing complexity by streamlining and defining standard processes is another area of potential. Data transparency and the consistency of data, as well as requirements management throughout the complete development cycle, are also significant.

Subsequently, an approach will be demonstrated to address these potentials and enhance the efficiency of the development process. In summary, there are two core factors that this work aims to address:

- Reduction of the time-to-market
- Transparency and traceability

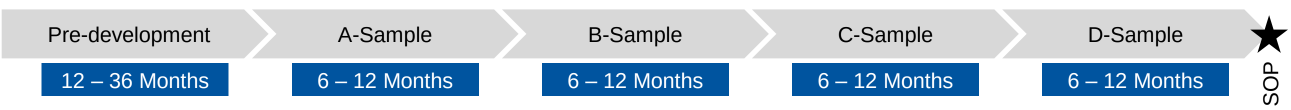


Figure 2: Estimated state of the art development duration

3. IMPROVED DEVELOPMENT APPROACH TO REDUCE TIME TO MARKET

The proposed development approach aims to reduce the time to market by providing a comprehensive overview of both the product development and production processes and highlighting the crucial linkages between them. By focusing on the seamless transition from identifying challenges to formulating and implementing solutions, we aim to streamline the entire development lifecycle, ensuring a more efficient path from concept to commercialization.

3.1 PRODUCT DEVELOPMENT PROCESS

The product development process visualized in figure 3 will be further explained by using phase definitions, sample definitions, and workstream definitions. The focus of this paper is the engineering process. Business development and other organizational departments are not part of this consideration.

3.1.1 PHASE DESCRIPTION

The overall product development process can be broken down into the overarching phases of **initiation** and **cell engineering**. These are followed by **iterations** of cell engineering for various samples (ranging from A- to C-Sample), along with the **pre-series** and r**amp-up phases**. The following sections will explain each phase in detail.

During the **initiation phase**, preparation for cell engineering occurs, involving defining key use case requirements. This entails teardowns and benchmarking to analyze existing products, requirements management to prioritize specifications, and patent analysis to ensure innovation and prevent infringement. Initial process requirements and concepts are also established, along with supplier pre-screening to identify potential partners and materials for the development phase.

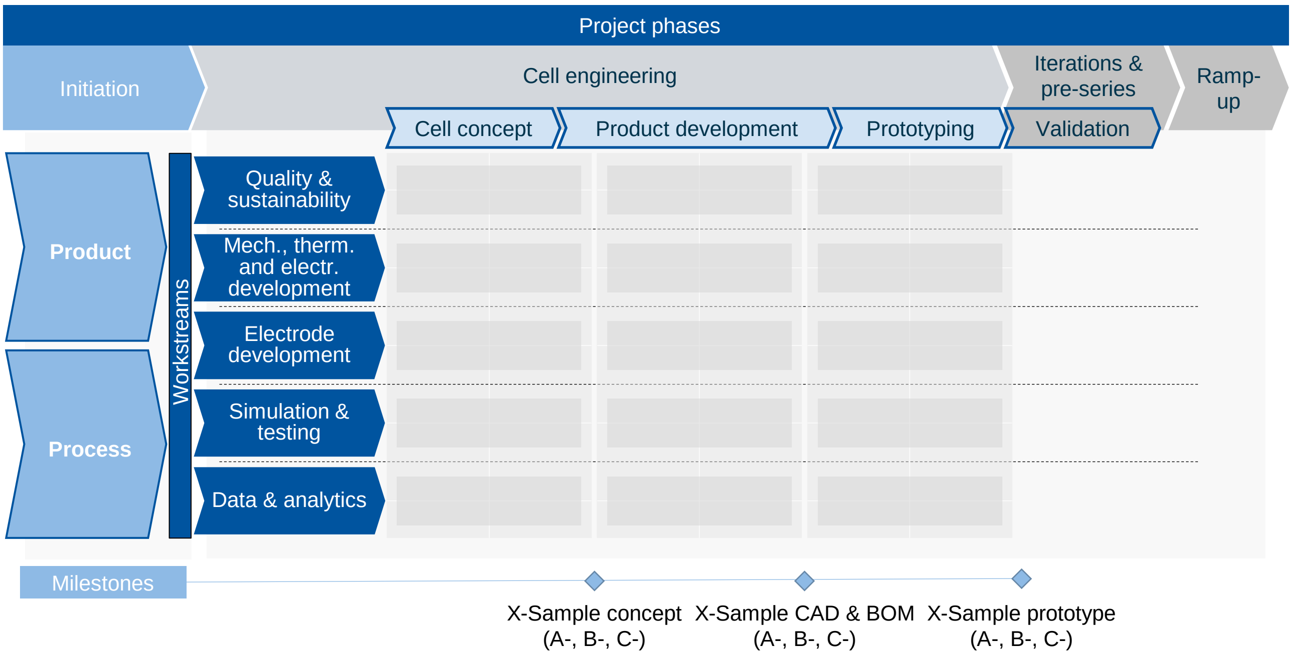


Figure 3: Product development process of battery cells

In the **cell engineering phase**, the core development takes place. Based on the requirements, concepts are developed and compared, which evolve into mature products through various sample iterations. Due to the extensive scope of this phase, the focus in the following sections will primarily be on cell engineering, with particular emphasis on the A-Sample phase. This phase targets the initial product concept and represents the most complex part of the development process. In the **pre-series phase**, the cells are produced on a series scale. The focus is on a detailed review of all relevant product factors. The phase ends with the start of production (SOP). In **the ramp-up phase**, the production capacity is increased, and the quality of the products is continuously monitored.

3.1.2 SAMPLE DESCRIPTION

During the development process, various sample phases are distinguished. In industry common samples are from A- to C-Sample. The proposed innovative development process is based on three sample phases, which are explained in more detail in the following. Within each of these sample phases, there are sub-phases that include cell concept, product development, and prototyping (see figure 4).

In the **A-Sample phase**, the first samples are produced with laboratory-scale equipment. The focus is on functional and independent component tests. The A-Sample represents the end of the development phase and does not yet focus on the service life and durability of the cell components. Usually, up to 500 A-Samples are produced. The **B-Samples** are produced using laboratory or pilot-scale systems, with a typical production volume of 10.000 to 20.000 units. The tests carried out include installation and functionality tests on test benches. The aim here is to confirm the function and predict the reliability. In addition, based on the B-Sample, a fundamental decision is made regarding in-house production or external procurement of the cells. The **C-Sample** with more than 20.000 samples is manufactured using pilot plants or near-series production plants. The cell design (e.g. surface quality) is designed for series production. The scope of testing places particular emphasis on overload conditions as well as functionality and durability at a higher system level.

Each of the sample phases is complemented by a validation phase, which begins during the prototyping phase and transitions into the cell concept phase of the subsequent sample phase

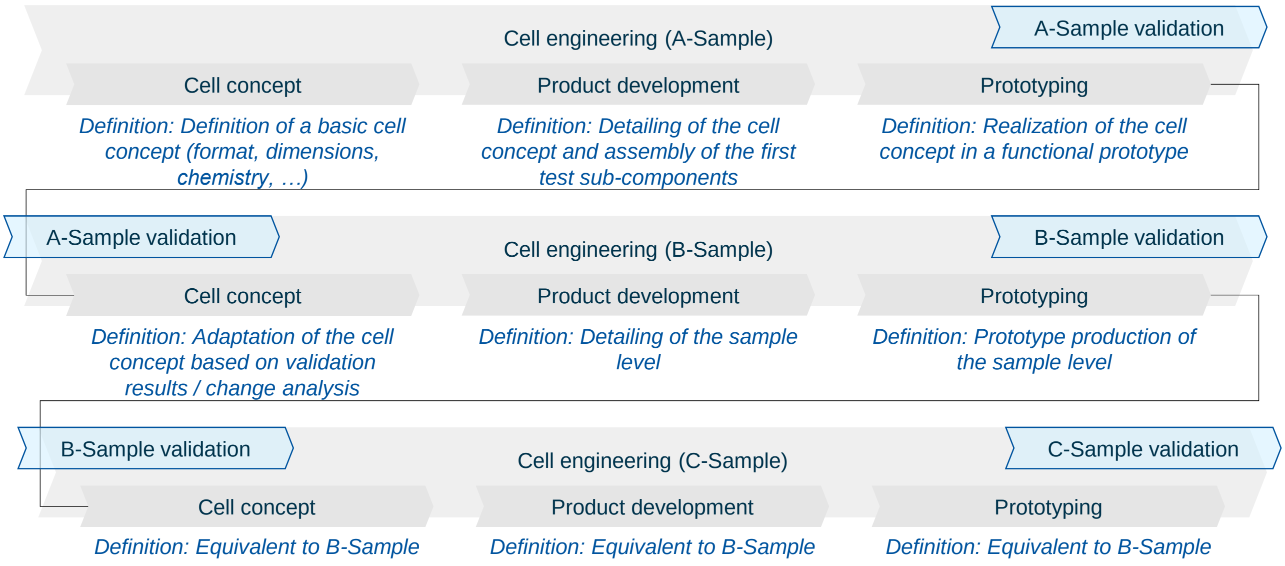


Figure 4: Sample description

As part of the validation, the functionality of the prototype or its components is tested, and necessary modifications for the following sample phases are derived. In this publication, our focus is particularly on the development of the A-Sample, highlighting its pivotal role in the iterative process of improvement and refinement.

3.1.3 WORKSTREAM DESCRIPTION

Each described phase of the development process is addressed through various so-called workstreams. In the context of this approach, the five distinct workstreams are divided into **requirements & quality, mechanical, thermal, and electrical development, electrode development, simulation & testing,** and **data & analytics.** To provide a better understanding, an overview will be given in the context of describing the procedures, key results and milestones, and key challenges and potentials. Further details can be found in figures 5-7. As already mentioned, the focus of this publication is on cell engineering of A-Sample battery cells.

In the **cell concept phase**, the complex solution space that arises from the requirements for the battery cell product and the communication between different areas represents a fundamental challenge for all workstreams. For this reason, early assessment of requirements fulfillment offers great potential for reducing the solution space.

As part of the cell concept phase, general requirements for the battery cell to be developed are derived from the initial customer requirements or specific end-use cases in the requirements & quality workstream. The initial framework for requirements management and the sustainability evaluation concepts and product characteristics for the basic cell design are defined as key results.

The mechanical, thermal and electrical development workstream is fundamentally focused on the development of the core cell design and a basic safety concept. As part of developing these two initial design concepts, the complex interactions between cell design and safety and the given requirements pose a particular challenge. Key results and milestones in the cell concept phase for this workstream represent a first version of the CAD model, the bill of materials (BOM), and the cost model in addition to the initially defined product properties.

Electrode development involves supplier screening and evaluation, which results in a supplier long list. A key challenge here is the consideration of material quantities for individual tests and prototypes. In addition, supply chain risks and second sources are also considered. In addition, the cell chemistries, electrolytes, additives, and binders as well as the electrode dimensions are preselected. On this basis, initial electrode target parameters are also calculated, such as the specific area capacity and mass loading.

In the simulation & testing workstream, the entire simulation and testing scope is defined, and initial basic (mechanical, thermal, electrical, and electrochemical) simulations are created. The challenge arises from the limited availability of highly material-specific data, which can potentially lead to high inaccuracies and complicates the evaluation of deviations of developed models from reality. Despite this, the development of initial simulations of the cell using data from teardowns offers great potential to accelerate the entire development process. The early development of such simulation models makes it possible to further develop the existing model in later development phases and, if necessary, to develop detailed models that deal with specific safety-related issues or new design decisions.

The data & analytics workstream involves the definition and initial provision of relevant tools and databases for product development. In addition, the state of technology is evaluated based on publicly available data and cell tests carried out in-house. However, the often-limited public database and imprecise customer requirements pose a challenge here. There is potential in ensuring a high level of data transparency, traceability and consistency. The definition and, in the subsequent phases, further development of a consistent end-to-end toolchain is a key result of this workstream, which is examined in more detail in chapter 4.

From the **product development phase** onwards, an early coupling of product and production process development across workstreams offers great potential to meet the challenge of the high overall complexity of product development up to the start of production. Coupling product and process simulation offers the opportunity to align product and process requirements at an early stage (see chapter 3.3).

As part of the requirements and quality workstream, the existing suppliers are evaluated in this phase regarding defined evaluation criteria. In addition, a final specifications sheet is defined for the A-Sample and the strategic decision regarding in-house production or external procurement is made.

In electrode development, specific material performance evaluations are carried out by setting up various test carriers with different initial electrode formulations. Electrode recipes are iterated and optimized for performance and producibility based on these results. Core challenges here include the lack of reproducibility of coin or laboratory cells and the lack of consideration of reproducibility in the production process on a series scale.

The simulation and testing workstream builds on the existing simulations, by carrying out tests with the developed test carriers and the data generated from them, and simulates further electrical, thermal, and structural chemical parameters. Furthermore, the development of initial performance models is started to simulate further quality properties of the final cell, such as capacitance and internal resistance. In addition, the initial coupling of product and process simulation mentioned above is a key result. This procedure is examined in more detail in chapter 3.3.

In the **prototyping phase**, initially defined key results are finalized and defined regarding the cell prototype for the A-Sample. Based on the BOM, the LCA approach is recorded as part of the requirements & quality workstream, and a specification sheet is defined through the final alignment of the A-Sample requirements. In mechanical, thermal, and electrical development, the BOM, the CAD, and detailed component drawings with detailed tolerances are recorded, while in electrode development the electrode design is finalized. The simulation and testing workstream focuses on the physical testing of the A-Sample prototypes in terms of performance, lifetime, and functional safety. In addition, the existing simulation models are refined and validated with the new data obtained. In particular, the initial estimation of production process parameters by coupling the product and process models represents a high potential for evaluating processability on a series scale. To this end, the data and analytics stream is developing an evaluation tool for processability.

Cell concept phase (A-Sample)

Workstreams	Procedure	Key results and WS milestones	Key challenges and potentials

Requirements & quality	+ General requirement generation
	+ Definition of quality parameters and sustainability evaluation concept for basic cell concept
		+ Initial requirements framework and key requirements quantified
		+ Sustainability evaluation concept
		+ Product features for basic cell design defined
			+ Challenges
			  + Breaking down system requirements to the cell level
			  + Assign/collect quality and sustainability criteria
			+ Potentials
			  + Factors influencing cost reduction (CO_2 price, recycling, maintenance)

Mech., therm. and electr. development	+ Development of basic cell design
	  + Cell format
	  + Cell dimensions
	  + Tab/connection design
	  + Passive safety devices & materials
	+ Development of cell safety concept
	  + Current interruption
	  + Current reduction
	  + Safety vents
	  + Thermal and electrical isolation
		+ Key product features and components specified based on:
		  + Basic cell design
		  + Cell safety concept
		  + Initial simulations
		+ Initial CAD model
		+ Initial BOM and cost model
			+ Challenges
			  + Complex interdependencies in-between cell design, cell safety concept and requirements
			  + Cost estimation

Electrode development	+ Supplier screening and evaluation
	+ Preselection of cell chemistry, electrolyte, additives, binder
	+ Initial calculation of the electrode target parameters
		+ Supplier long list
		+ Estimated specific area density
		+ Preselected:
		  + Cell chemistry
		  + Electrolyte
		  + Additives
		  + Binder
		  + Electrode dimensions
			+ Challenges
			  + Compatibilities in-between the electrode components
			  + Supplier selection in consideration of material quantity for prototypes, supply chain risk and 2nd sources)

Simulation & testing	+ Definition and planning of simulation and testing scope:
	  + Cell behavior characterization
	  + Cell behavior validation
	  + Validation data
	+ Initial basic simulation models (mechanical, thermal, electrochemical)
		+ Simulation and testing plan
		+ Cell dimensioning tool
		+ Initial simulation results
			+ Challenges
			  + Evaluation of the deviation of models from reality
			  + Material specific data availability
			+ Potentials:
			  + Initial simulations of the cell model
			  + Estimation of requirement fulfillment
			  + Simulation input through teardowns

Data & analytics	+ Definition of tools and needed databases
	+ Benchmarking / Teardowns
	+ Evaluation of the state of technology
	+ Data Analysis
		+ Simulation and testing plan
		+ Cell dimensioning tool
		+ Initial simulation results
			+ Challenges
			  + Limited publicly available data basis
			  + Inaccurate customer requirements
			  + Complex solution space for requirements
			+ Potentials
			  + Data transparency and traceability
			  + Data consistency

Across all workstreams:

+ Challenges:
  + Complex solution space for requirements
  + Interfaces/communication between the individual areas
+ Potentials:
  + Early assessment of requirements fulfillment to reduce the solution space

Figure 5: Cell concept phase (A-Sample)

Product development phase (A-Sample)

Workstreams	Procedure	Key results and WS milestones	Key challenges and potentials

Requirements & quality	+ Definition of supplier evaluation criteria
	+ Conduction of a material performance and sustainability screening
	+ Conduction of a supplier cost evaluation
	+ Extension of the requirements to include initial production process requirements
	+ Evaluation of the strategical decision to produce in-house or to procure the cells externally
		+ Supplier evaluation criteria
		  + Material/component sustainability evaluation
		  + Material/ component performance evaluation
		  + Material/ component cost evaluation
		+ Final specification sheet for the A-Sample
		+ Strategical decision regarding in-house production or external procurement of the cells (make-or-buy)
		+ Initial LCA results
			+ Challenges
			  + Breaking down system requirements to the cell level
			  + Assign/collect quality and sustainability criteria
			+ Potentials
			  + Factors influencing cost reduction (CO_2 price, recycling, maintenance)

Mech., therm. and electr. development	+ Detailing the initial cell design and cell safety concept
	  + Extension by tolerances
	  + Concretization of the design based on technical production process restrictions
	+ Manufacturing/Acquisition of individual components
		+ Detailed cell design and safety concept
		  + Tolerances
		  + Design restrictions based on the production processes
			+ Challenges
			  + Complex interdependencies in-between cell design, cell safety concept and requirements
			+ Potentials
			  + Mechanical assessment of product/process coupling

Electrode development	+ Conduction of a material performance screening
	+ Test carrier production for the initial electrode formulations
	  + Coin cells
	  + Single layer pouch cells
	  + Multi layer pouch cells
	+ Determination of a favored electrode formulation
		+ Material performance evaluation
		+ Defined electrode formulations
			+ Challenges
			  + Reproducibility of the coin cells
			  + Lack of consideration of production processes on a series scale
			+ Potentials
			  + Chemical assessment of product/process coupling

Simulation & testing	+ Further simulation of electrical, thermal and structural chemical parameters with focus on specification and reparameterization
	+ Conduction of initial lifetime and safety assessments
	+ Test carrier testing
	+ Development of initial performance model
	+ Initial factory/production simulation
		+ Test cases of test carriers carried out and documented
		+ Initial thermal simulation carried out (temperature distribution/spread)
		+ Initial performance model set up (estimation of capacity, OCV, internal resistance, ...)
		+ Initial factory/production simulation defined
		+ Simulation models initially validated
			+ Challenges
			  + Quality of the test data
			  + Scalability of the simulation models
			  + Partially long test protocols
			+ Potentials
			  + Coupling process/product improves parameter specification
			  + Partial validation by coin cell

Data & analytics	+ Characterization of materials and data generation for further simulations
	+ Development of a standardized electrode evaluation tool
	+ (Screening and elaboration of AI and Tools for chemistry development)
		+ Detailed databases
		  + Addition of collected material data
		  + Addition of test carrier testing data
		  + Initial production process parameters
		+ (Defined AI and tools for chemistry development)
			+ Challenges
			  + Limited publicly available databases
			+ Potentials
			  + Data consistency
			  + Standardized electrode evaluation tool
			  + Use of AI based tools for chemistry development

+ Challenges:
  + Complex solution space for requirements
  + Interfaces/communication between the individual areas
+ Potentials:
  + Early assessment of requirements fulfillment to reduce the solution space
  + Early product and process coupling

Figure 6: Product development phase (A-Sample)

Prototyping (A-Sample)

Workstreams	Procedure	Key results and WS milestones	Key challenges and potentials
Requirements & quality	+ Alignment with further production requirements + Final alignment of the A-Sample requirements + Detailing of initial LCA results	+ Specification sheet for A-Sample + LCA approach for the A-Sample cell	+ Challenges + Limited data basis for sustainability indicators along the supply chain + Potentials + Early determination of sustainability factors + Consistency of requirements management
Mech., therm. and electr. development	+ Optimization of initial BOM and cost model + CAD model optimization based on prototyping experience	+ BOM + Cell cost model + Frozen product features (A-Sample) + Assembly drawings + Component drawings with detailed tolerances + Producable CAD / production CAD	+ Challenges + Combination of the various subcomponents into prototypes + Potentials + Early functional and requirements validation through prototypes
Electrode development	+ Assembly of large format pouch cells + Process parameter optimization for large format pouch cells	+ Finalization of the A-Sample electrode design + Recipe + Process parameters + Frozen electrode features (A-Sample)	+ Challenges + Producibility in series scale and equipment + Potentials + Chemical assessment of product/process coupling
Simulation & testing	+ A-Sample testing (focus: performance and lifetime) + Quantified comparison of test data with regard to specifications + Reparameterization of the models + Refinement of factory/production simulation (coupling of structural parameters) + Conduction of functional safety tests + Conduction of cell assembly test	+ Test cases A-Sample performed and documented + Factory/production simulation refined + Parameters updated based on tested A-Sample + Simulation models "25% version" (based on A-Sample) validated	+ Challenges + Low prototype production quantity + Quality of the test data + Scalability of the model + Potentials + End-to-end toolchain + Estimation of process parameters + Validation of the requirements
Data & analytics	+ Development of a tool to evaluate the processability of the defined A-Sample specification	+ Evaluation tool for the processibility	+ Challenges + Complex solution space for requirements + Potentials + Data transparency and traceability + Data consistency

+ Challenges:
  + Complex solution space for requirements
  + Interfaces/communication between the individual areas
+ Potentials:
  + Early assessment of requirements fulfillment to reduce the solution space
  + Early product and process coupling

Figure 7: Prototyping phase (A-Sample)

3.1.4 PHASE MILESTONES

To better understand the various phases, milestones are assigned to track development progress. These milestones act as checkpoints, highlighting significant achievements or transitions, ensuring the process stays on schedule and aligns with project goals. Each cell engineering phase includes three distinct milestones: "Sample concept", "Sample CAD & BOM", and "Sample prototype" as illustrated in figure 8.

Sample concept: The A-Sample concept represents the completion of conceptual development and the preliminary selection of the production process. This development covers key aspects such as selecting the production chain to define manufacturing steps, gathering relevant data and methods for guiding development, defining product features to outline capabilities and functionalities, establishing basic mechanical design and safety parameters, and choosing chemical and material parameters. Battery parameters are also set based on current technology and teardown insights. Unlike the A-Sample, the B- and C-Sample concepts evolve based on feedback from previous validation phases.

Sample CAD & BOM: For the A-Sample, this milestone is marked by a detailed cell concept supported by a fully developed CAD and a comprehensive BOM, incorporating all necessary data and methods for precise design, including safety parameters with specific tolerances and considering production process-related product limitations. The B- and C-Samples aim to refine the sample to a level ready for prototype production.

Sample prototype: In the A-Sample phase, the prototype is a functional model designed for validation and real-world testing. It includes frozen product features specific to the A-Sample, documented in a product feature database and CAD formats. The BOM is also finalized, ensuring consistency in materials and components. The development and validation of the prototype are informed by testing results, ensuring functionality and reliability. The B- and C-Sample phases focus on prototypes that demonstrate the sample level, prepared for more testing and refinement.

Furthermore, these milestones also serve as defined points in the development process to exchange information and results from preceding phases with other areas, such as production planning. Similarly, information from these other areas can be gathered as input for upcoming development phases. Accordingly, requirements and information from production planning can also be gathered here as input for upcoming product development phases. A coupling of product development and process planning will be further explored in chapter 3.3. The following chapter will examine the production processes of lithium-ion battery cells to give an insight into the complex production chain, which poses a fundamental challenge for production planning.

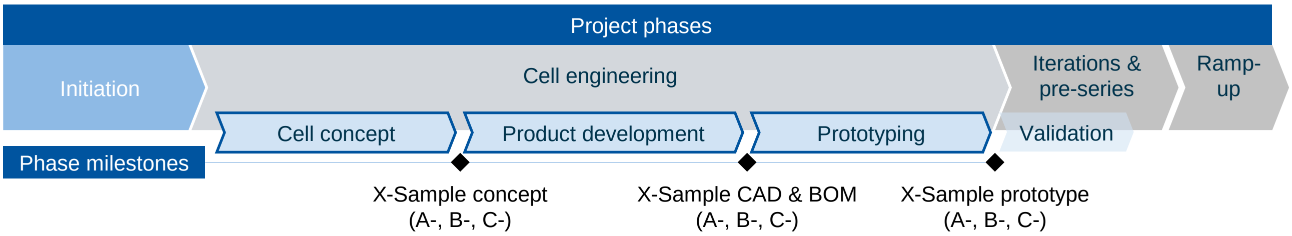


Figure 8: Phase milestones

3.2 BATTERY CELL PRODUCTION PROCESS

The production process for lithium-ion battery cells is a combination of a wide variety of production technology/engineering processes, resulting in a complex process chain. This results in a large number of interdependencies between information and parameters of the production process and the (intermediate) product itself, most of which are not fully understood.[3,4]

The conventional production process for lithium-ion battery cells can be divided into three overarching sections: electrode manufacturing, cell assembly and cell finalization. Each section can be further divided into several processes. Depending on the selected cell format, the production process steps in cell assembly differ in particular. Figure 9 shows an example of the production process for a pouch cell, which is explained in more detail in the following.[5,6]

Electrode manufacturing usually takes place on two separate lines for the production of anodes and cathodes. First of all, the corresponding active materials are mixed with solvents, binders and other additives during the mixing process and processed into the electrode slurry. The slurry is then coated on both sides of a current collector foil. Copper foil is usually used for anodes while aluminum foil is preferred for cathodes. The coated foils are subsequently dried to remove solvents. The dried electrodes are then compressed by rotating pairs of rollers during calendering to achieve the defined final layer thickness and porosity of the electrodes. During slitting, the large electrode coils are then separated into smaller coils whose size depends on the defined electrode and cell design. Finally, these smaller coils are stored in vacuum furnaces to remove the residual moisture. [5,6]

In cell assembly, the defined shapes and sizes are separated from the electrode coils. Subsequently, the individual cathode and anode sheets are stacked alternately with a separator film in between. The number of layers to be stacked depends on the cell design. Then, the uncoated current collectors of the individual stacked electrode sheets are cut to size and welded to a metallic tab. The cell stack is then placed in deep-drawn pouch foil and partially sealed. Finally, electrolyte is injected into the pouch foil with a dosing lance, and the pouch cell is finally sealed.[5,6]

Cell finalization represents a highly variable process stage in which the sequence and number of sub-process steps to be carried out can be highly individualized. Optionally, at the beginning, a pre-treatment of the cells can be performed to accelerate the distribution and penetration of the electrolyte into the pores of the electrodes and separator. For example, cells may be stored at defined pressures or temperatures for this purpose. As part of the formation process, the initial charging and discharging of the cells are carried out according to defined current and voltage profiles. This forms the solid electrolyte interface layer, which acts as a boundary layer between the electrolyte and the anode. During the initial charging process, gas is generated, which is collected in a gas pocket in pouch cells and then removed. While prismatic cells are typically degassed via the temporarily closed filling opening, this step does not usually take place with cylindrical cells due to their size and therefore small amount of formed gas. In the subsequent aging process, the cell is monitored for its electrical properties and potential defects under specific environmental conditions. Finally, the cell undergoes End-of-Line (EOL) testing to evaluate its performance properties and categorize it accordingly. [5,6]

Understanding the intricate interdependencies in-between the intermediate products, the final product, and the various influences of the production processes is crucial for an efficient design of the battery cells as well as the corresponding production processes. These relationships encompass multifaceted dynamics that influence critical factors such as quality, costs, and lead times. There is potential for improvement in battery cell production in all of these areas. In this context, the use of simulation and data-based approaches represents an opportunity to better understand and describe the complex relationships. In this context, the use of simulation and data-based approaches represents an opportunity for discerning patterns and correlations and thus, to better understand and describe the complex relationships. The acquisition and structuring of relevant information is a fundamental step for the use of these approaches, providing a structured framework, for comprehending the intricate correlations. [4,7,8]

Structural parameters: All quality parameters of used materials and components, as well as intermediate products, that represent their physical properties and therefore influence the performance parameters of the final cell (e.g., particle size distribution, wet layer thickness, porosity).

Performance parameters: All quality parameters, that define the performance of the final battery cell (e.g., self-discharge rate, energy density).

Process parameters: All machine parameters that can be directly adjusted during the production processes in order to impact the structural properties of the (intermediate) product (e.g., mixing speed, coating web speed, and drying temperatures).

Equipment feature: All machine parameters that can not be changed on short notice and are defined by equipment or tool design (e.g., mixing tank volume, slot die width, and length of the drying line).

Ambient parameters: All parameters that define the conditions prevailing in the production process environment are ensured by room conditioning systems (e.g., humidity, ambient temperature). [4,7,8]

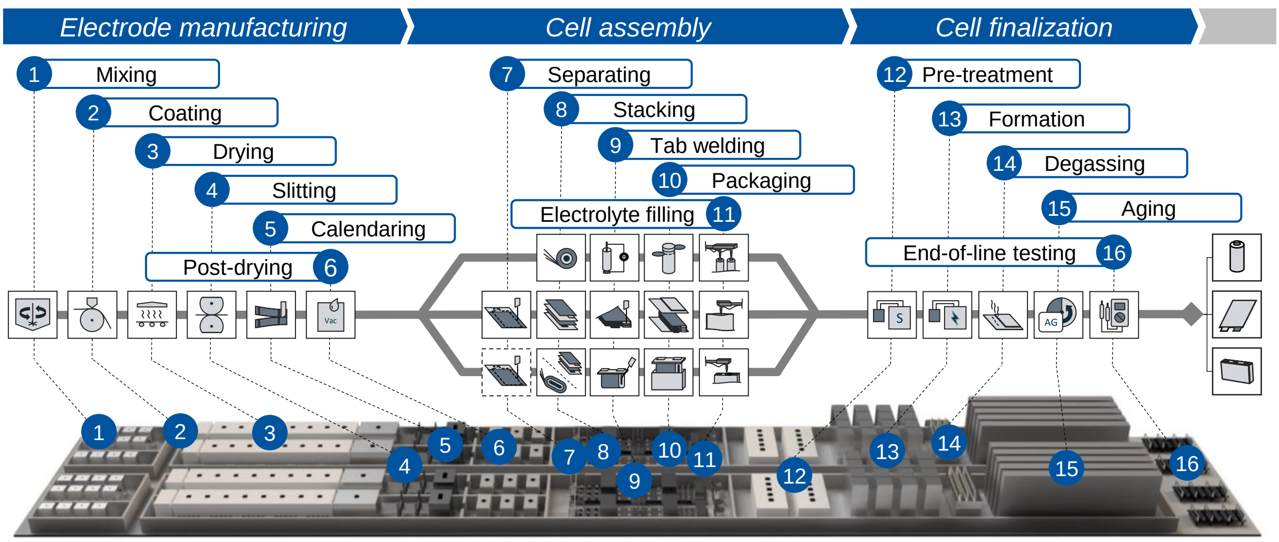


Figure 9: Production process of lithium-ion battery cells

3.3 PRODUCT AND PROCESS LINKAGE

In the previous chapters, the product development process and the production process have already been explained in detail. Now, the linking of product and process is introduced. The interconnection is crucial to prevent delays during ramp up due to production challenges that were previously overlooked. The general methodology visualized in figure 10 is explained with focus on the process steps coating and drying with specific examples of the linking strategy.

Milestones serve as critical checkpoints to ensure the seamless integration of product development demands with production timelines for battery cells. These are not just markers of progress but as opportunities for synchronization and alignment between the envisioned product and its manufacturability. As already mentioned before the relevant milestones are sample concept, sample CAD & BOM and the sample prototype. Each milestone for the cell engineering phases from A- to C-Sample. For each milestone, performance parameters are derived from the product requirements. However, the performance parameters can also necessitate an adjustment of the product requirements.

Based on the performance parameters, the respective structural parameters of the full cell that are required to achieve these properties can be derived. These structural properties of the full cell in turn define the target for the production process chain. The process parameters of the highly coupled process steps must be selected in such a way that they lead to the desired structural parameters of the individual process steps and ultimately along the entire process chain to the specified structural parameters of the full cell.

Innovative is the early addition of simulations to conventional testing to determine both the structural parameters of the full cell, as well as the structural and process parameters along the process chain. By using simulations, the extent of the conventional testing can be reduced, thereby shortening the development time. Simple interactions can be directly linked without simulation and testing.

The actual product/process coupling takes place via the structural parameters, which in turn depend on the process parameters. While the structural parameters of the full cell serve as input and therefore as connection between the process chain and the product model, the structural parameters of the intermediate product connect the individual

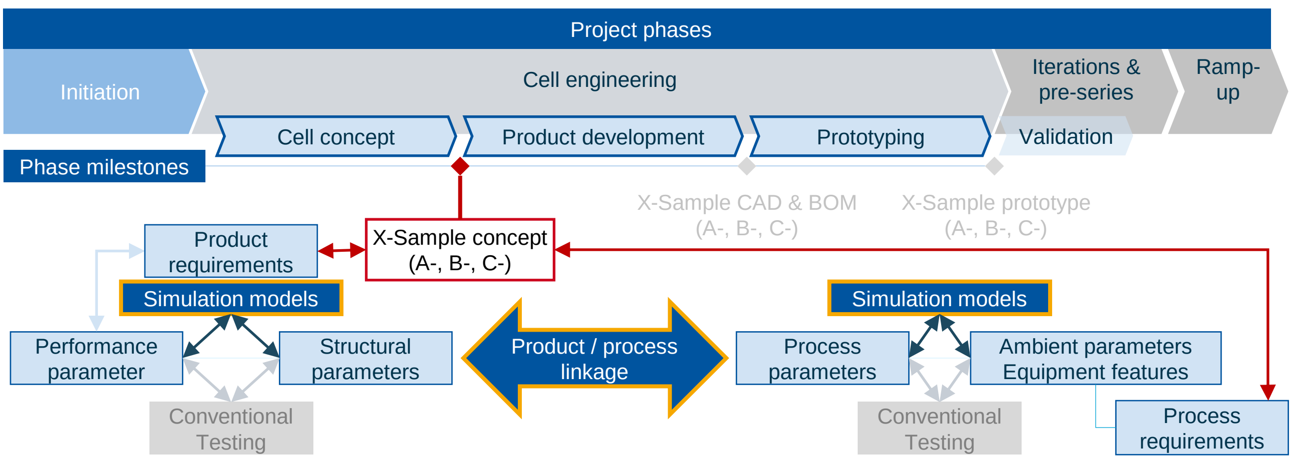


Figure 10: Product and process linkage

process steps. The relation between input and output structural parameters of each process steps at this is determined by the process parameters.

Simulations can also reduce the effort required to derive ambient and equipment features from process parameters on the production side of the linkage. Finally, process requirements can be derived from the equipment features, as well as ambient and process parameters. These additional process requirements can be incorporated into the upcoming production planning phase. Likewise, the coupling can define new product requirements based on process requirements, narrowing the solution space early on.

An example of the simulation-based coupling of product and process requirements for lithium-ion battery cells is explained below, focusing on electrode production resulting from the coating and drying process.

A key performance parameter derived from customer requirements for battery cells is the target energy density. The coating layer thickness of the electrode slurry on the current collector film significantly influences energy density and serves as a critical quality characteristic of the intermediate product electrode. Early simulation model development during the cell concept phase allows estimation of the necessary layer thickness using knowledge from literature and in-house teardowns, minimizing reliance on conventional test data. During the product development and prototyping phase, the results from the test carrier and prototyping test runs can be used to continuously improve the simulation models.

Achieving the desired layer thickness during coating is crucial and depends greatly on the electrode slurry's volume flow and the web speed during coating and drying. Production process simulations, based on coating thickness values and initially selected formulations can be used to approximate the dependency of relevant process parameters on targeted structure parameters. The early use of physical models is particularly useful to substitute physical production runs. Further detailing of production process models is then carried out using pre-series and ramp-up production runs.

Process requirements also influence the production process design, affecting application system selection and equipment design like slot dies. Using production process simulations improves equipment feature decision-making, imposing new demands on the production planning processes.

Early derivation of production planning requirements' influence on product design is vital. For instance, drying section length may be constrained by available space, impacting web speed, volume flow, and electrode layer thickness, potentially affecting not only electrode quality but also overall cell design.

Understanding and optimizing interdependencies between parameter types are crucial for effectively tailoring battery cell designs and production processes, ensuring performance targets, maintaining product quality, and enhancing production efficiency.

4. DIGITAL END-TO-END TOOLCHAIN TO SUPPORT CELL DEVELOPMENT

4.1 DEFINITION AND OVERVIEW

An efficient approach to reducing time to market is an end-to-end toolchain to support the process digitally. An end-to-end toolchain is a set of digital tools that are linked together in such a way that a seamless transfer of necessary data and information along the complete cell development process, including the manufacturing process chain, is possible by clearly defining the individual interfaces between the applications. This includes, for example, simulation and analytics applications, databases or software for product life cycle management. Such a holistic approach enables a defined determination and transfer of the necessary information for the coupling of product and process simulations.

Figure 11 shows an example of a linked toolchain during all project phases from the initiation phase up to ramp up. The tools can be clustered into different categories. The graphic shows an excerpt of the most important tools to provide an understanding of the methodology. It distinguishes between lifecycle management, databases, simulation, and analytics. The various tools have defined input and output parameters so that the coupling of multiple sub-models are possible without any issues. Simulation, for example, uses data from different databases to build up the knowledge base of the models. Such a toolchain enables a highly transparent approach to have a clear structure of available data and data transparency throughout the whole process. With a focus on the presented methodology, it is possible to define performance and process parameters and link them together at the defined milestones in early phases of product development. In doing so, not only product data but also process data (especially for the transfer from A-Sample to series production) are considered.

4.2 DEEP DIVE: END-TO-END THERMAL SIMULATION

The end-to-end use and further development of a digital toolchain along the product development process is considered in more detail below using the example of thermal simulation, which is illustrated for the A-Sample in figure 12. The cell heating behavior description can be based on data driven, electrothermal or electrochemical approaches. In practice the user needs to decide on a phase specific approach in relation to available input data

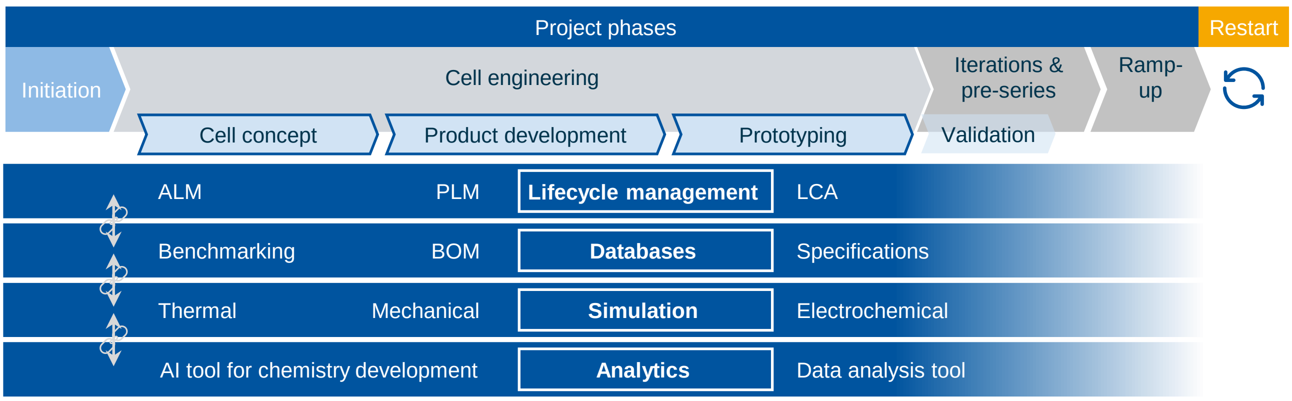


Figure 11: End-to-end toolchain

and computational resources. Based on the general customer requirements from the initiation phase, the key requirements for thermal safety and thermal design can be derived: These generally include maximum permissible temperatures, maximum temperature gradients, maximum C-rates and the service life of the battery. Optionally, requirements for the cooling system to be used in the battery system can already be specified here.

As part of the cell concept phase, the core requirements are supplemented with information from the other workstreams that run in parallel to the simulation and testing stream. In addition to the initial design decisions regarding mechanic cell design and cell safety, databases based on literature values and information from teardowns are used. Based on the information available so far, the electrothermal simulation and testing scope is defined first.

This corresponds to the specification of which simulation models are to be set up in addition to the overall cell model to examine individual components in depth regarding their thermal design. Subsequently, initial simulation models are set up according to the defined scope. The simulation result support concepts decisions such as stack orientation, mechanical component dimensions or optimal cooling strategies based on cell geometry.

An example of a typical electrothermal simulation result during concept phase is shown in figure 13 where the optimal cooling strategies are analyzed in parallel to different mechanical cell configurations (6 tabs, 8 tabs and tabless design) for 4680 cells. Based on the initially created electrothermal simulation models, the first virtual thermal validation of the initial cell design regarding temperature profile and charging capability is carried out. This allows for

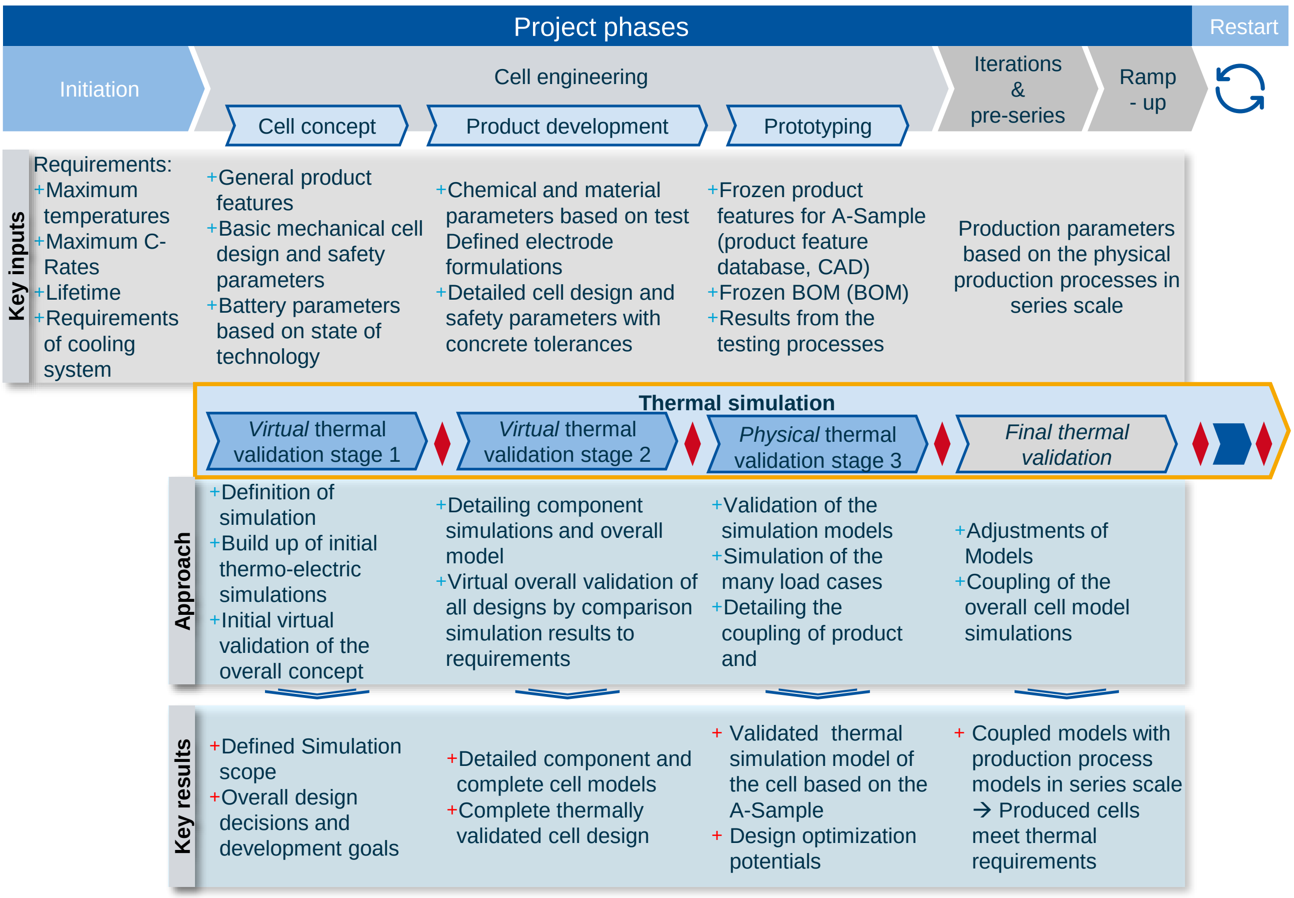


Figure 12: Thermal simulation

the derivation of terminal positions, maximum electrode losses, and optimal cooling approaches for the battery cells.

The second virtual validation takes place during the Product development phase. The initial simulation models are supplemented by cell design behavior parameters (e.g., thermal stack heat conductivity, electrical direct current resistances for various conditions). Additionally, these tests yield specific electrode formulations and production planning constraints, aiding initial product process planning as part of the first milestone. Newly acquired data refines initial simulation models, validating design decisions for the first product sample. Deeper examinations may focus on subcomponent models or address specific thermal issues; for instance, losses in electrodes can create hot spots within the battery cell. Manual adjustments via testing trials are time-consuming and costly compared to simulations.

Physical thermal validation is now carried out in the prototyping phase. Here, the simulation results created are validated by physical tests using the prototype of the A-Sample. Furthermore, the coupled product and process models can be further detailed using the findings from the physical tests.

Simulations are also used for load cases that cannot be carried out physically or only with great effort. For example, the number of high-current tests can be reduced using simulations. Finally, the validated thermal simulation models are obtained in this phase, as well as further optimization potentials for the cell design, which are based on the physical tests and final simulation results. The results also serve as input for models from module and system development.

In further iterations of the cell engineering process for the following cell samples, focused design questions and iterations can be again supported via electrothermal simulation, and the module and pack development and simulation can be supplied with input data.

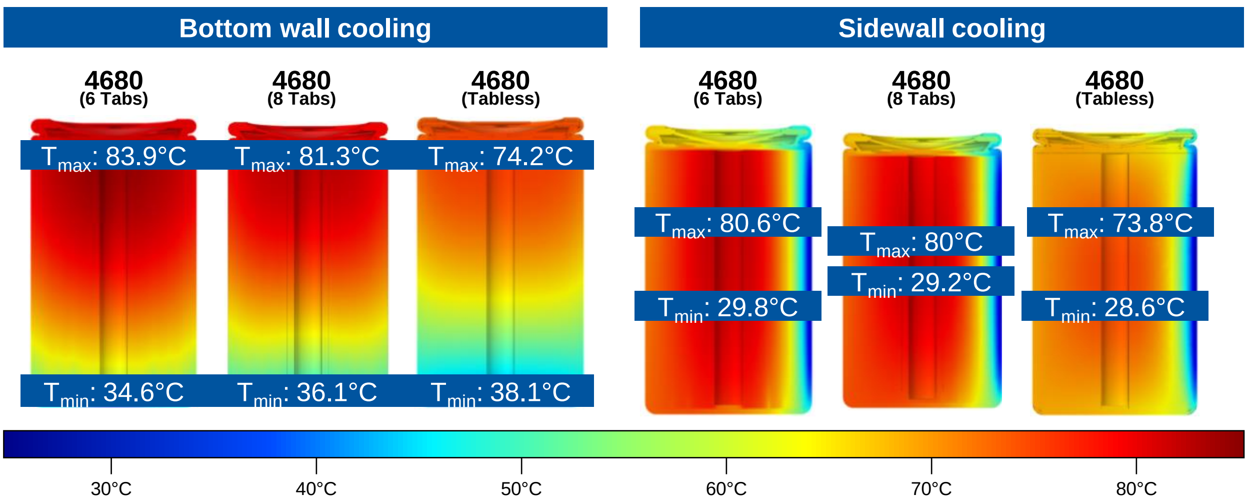


Figure 13: Comparison of bottom and sidewall cooling for steady state results for 3C continuous charging and identical cooling loop efficiency[9]

5. CONCLUSION AND OUTLOOK

Batteries are and will remain an essential success factor for electromobility and climate protection through sustainable energy supply. In the industry, there is a high demand for optimization and enhancement of efficiency in the development of battery cells. The Technology Cluster Battery Cell as a cooperation within industry and research has set itself the task of exploiting potential and identifying new approaches. The overarching goal is to reduce the time to market and decrease costs. Within the scope of the publication, challenges and potentials in development were initially presented, followed by the introduction of an innovative approach that addresses these issues. The approach is mainly based on a structured product development process with a continuous linkage to battery manufacturing processes. Beside the structure itself an approach for an end-to-end toolchain is presented with a deep dive in thermal simulation. It shows the potential of digital tools within the product development of battery cells. In summary, four key impacts to reduce time to market and cost could be identified. These are also summarized in figure 14.

1. Standardized procedures: In industry, currently, many different approaches are used for cell development without a clear definition of the interfaces between departments. Often series development models are used with a lack of validation in early development stages. This often leads to unexpected delays in project progress and inestimable scopes for necessary changes. The overall complexity of product development can be reduced by means of a predefined product development process with specific milestones. In addition, the specification of concrete key results helps to exchange information between individual departments and reduce delays in development.

2. Early coupling of product and process: The collaboration between development and production is not yet established in the early phases of development. This leads to unnecessary delays and lack of synchronization. The implementation of early coupling helps to align product and production process requirements and reduce the complex solution space at an early stage. In particular, the use and coupling of different simulations offers great potential in this field.

Key Impacts
to reduce time to market and cost

1 **Standardized procedures** enable efficiency improvements and simplify the process between departments.

2 **Early coupling of product and process** enables integrated development and avoids later necessary adjustments due to process errors and further iterations.

3 **Early simulation** allows validation during development even without prototypes.

4 **Consistency and transparency of data and requirements** enable targeted development with standardized procedures and avoid unnecessary repetitions and adjustments.

Figure 14: Key impacts to reduce time to market and cost

3. Early simulation: Early simulation allows validation during development even without prototypes: Early use of simulations for partial validation of concepts allows for the elimination of prototypes, reduction of testing scope, and the optimization of early design ideas during product development. Furthermore, the coupling of different simulation models such as product and process simulations offers a great potential to reduce the complex solutions space to fulfill all requirements.

4. Consistency and transparency of data and requirements: Enable targeted development with standardized procedures and avoid unnecessary repetitions and adjustments: Consistency and transparency are often lacking because various stakeholders use different data sources and there is no single source of truth. Data that would provide early transparency of the concepts are frequently missing.

In addition to a standardized and accelerated battery cell development process, there are other key factors for improving e-mobility. In particular, the further digitalization of processes is arousing great interest in the industry. In connection with the technology cluster, further activities are planned in the investigation of detailed simulation models for an end-to-end toolchain and looking at quality improvement potentials in battery production.

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AUTHORS

PEM | RWTH Aachen University

Prof. Dr.-Ing. Achim Kampker
University Professor & Founder
PEM | RWTH Aachen University

Prof. Dr.-Ing. Heiner Heimes
Member of Institute Management
PEM | RWTH Aachen University

Moritz Frieges
Chief Engineer
PEM | RWTH Aachen University

Benedikt Späth
Research Associate
PEM | RWTH Aachen University

Rui Yan Li
Research Associate
PEM | RWTH Aachen University

Jonas Gorsch
Research Associate
PEM | RWTH Aachen University

Robert Ludwigs
Research Associate
PEM | RWTH Aachen University

Capgemini

Michael Müller
Head of Climate Tech & Sustainability
Capgemini

Marcus Fiege
Head of Center of Excellence Battery
Capgemini

Dr. Christoph Weißinger
Virtual Battery Development Lead
Capgemini

Moritz Brüßler
Simulation Expert
Capgemini

Jens Radtke
Battery Development Expert
Capgemini

Niklas Drope
Simulation Expert
Capgemini

Marco Schleeh
Digitalization Expert
Capgemini

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Production Engineering of E-Mobility Components
RWTH Aachen University
Bohr 12 | 52070 Aachen

Phone **+49 241 8023029**
E-mail **info@pem.rwth-aachen.de**
Web **www.pem.rwth-aachen.de**

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CONTACT

Prof. Dr.-Ing. Achim Kampker

University Professor & Founder

info@pem.rwth-aachen.de

Production Engineering of E-Mobility Components

RWTH Aachen University

Bohr 12 | 52072 Aachen

www.pem.rwth-aachen.de

Michael Müller

Head of Climate Tech & Sustainability

michael.c.mueller@capgemini.com

Capgemini Engineering

Frankfurter Ring 81 | 80807 München

www.capgemini.com