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Developing a concept for the implementation of predictive quality in battery production

Achim Kampker, Heiner Heimes, Paul Lingohr*, Jessica Schmied, Henning Clever, Benjamin Dorn

Chair of Production Engineering of E-Mobility Components (PEM) of RWTH Aachen University, Aachen, Germany

* Corresponding author. E-mail address: p.lingohr@pem.rwth-aachen.de

Abstract

The supply of batteries plays a crucial role in the electrification of the automotive industry and thereby in reducing CO₂ emissions. With strict regulations forcing the ban of internal combustion engines and the reduction of emissions, the demand for batteries has risen drastically. In current battery productions, planned production volumes are in most cases not reached due to high scrap rates. Reasons for this lay in the lack of predictability of product quality due to process complexity and interdependencies both on the process level and on the parameter level. The reduction of scrap through data-driven methods in battery production offers the potential to increase production volumes addressing the global demand and to preserve energy and materials. Tackling the challenge of high scrap rates, existing and conventional methods in quality management lack the applicability in complex processes and the predictability of product quality. Predictive quality describes an industry 4.0 application and the approach to use production data to predict process and product related quality characteristics. In this paper, a concept for the technical implementation of predictive quality in battery production is developed. For this, an overarching concept is outlined and based on this the technical infrastructure described. The concept highlights the required data collection as well as data processing and addresses the development of prediction models. By applying the developed concept, the deployment of quality prediction models and the detection and compensation of scrap at an early stage is enabled.

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1. Introduction

The automotive industry has been undergoing a transformation towards electrification, with the lithium-ion battery playing a critical role in enabling this paradigm shift. The success of this transformation is contingent on the ability to meet the forecasted demand for traction batteries. By 2030, it is projected that demand for traction batteries in the automotive industry will exceed 3.100 GWh per year with an annual growth rate of 30 % [1]. In 2021, global production

capacity was still at 706 GWh per year, which rises the issue of scaling battery production [2].

Closing the gap between demand and production capacity significant challenges associated with setting up and operating battery productions need to be overcome. This is particularly evident in the scrap rates of up to 10 % in series production and even higher values in the start-up phases of battery production [3, 4]. The primary causes are the complexity of battery production with many different processes, the risk of consequential defects and the lack of reworkability.

Industry 4.0 approaches offer a solution for the challenges in battery production by utilizing the data generated in the production process [5]. For this, battery production is particularly qualified, as very large amounts of data are generated, especially in giga-scaling with very short cycle times and high production volumes. By analyzing the generated data in real time, data-driven solutions aim to improve efficiency, quality, and productivity by gaining insights into process and product characteristics. [6]

In this context, predictive quality describes a data-driven solution, which utilizes the generated data during production to make a prediction about the quality characteristics in the end [7]. This approach can be applied to single processes or process sections predicting intermediate products or to the complete process chain predicting final cell characteristics. Predictive quality offers several benefits, particularly in battery production. It enables the reduction of scrap by detecting quality deviations early in the process and rejecting intermediate products before the production process is completed. For example, defective electrodes can be rejected during separation. The integration of feedback loops also enables direct process optimization by adapting parameters based on the predicted quality characteristics. Additionally, it can preserve resources by avoiding the production of complete cells with defective components, leading to lower energy and material consumption, and simplified recycling.

This paper shows how the challenges in battery production, such as high scrap rates, can be answered by data-driven methods. In particular, the concept of predictive quality offers significant potential for optimization of the battery production. This paper discusses the current state of the art for the implementation of data-based solutions and presents a concept for the implementation of predictive quality in battery production. The implementation of predictive quality in battery production is explained as well as finally summarized and discussed.

2. Challenges in battery production

Due to the rising demand for battery cells new gigafactories with a capacity of up to 4.200 GWh per year are planned until 2030 in Europe [1]. New players, including start-ups and automotive OEMs, are entering the battery production market alongside established manufacturers. This creates an additional challenge due to their limited knowledge of battery production. However, the complex and long process chain in battery production poses a significant challenge for manufacturers [8, 9]. Battery production is structured in electrode manufacturing, cell assembly, and cell finalization [9, 10]. Each stage comprises a variety of materials and processes, ranging from mechanical processes to substantial alteration to electrochemical reactions, and requires different production environments, such as dry rooms. [8, 11]

The complexity in battery production results in various production-related challenges, such as the risk of error concatenation due to the long process chain. Additional issues are the lack of rework possibilities of intermediate products in the production process and the strong link between cell quality and the characteristics of the production process. Overall, this

results primarily in scrap rates of up to 10 % in series production and even higher rates during production ramp-up [3, 4]. The highest scrap rates are found in the process steps of coating in the area of electrode production and stacking in the area of cell assembly [12]. The high reject rates are particularly critical in electrode manufacturing, as the electrodes account for 39 % of the total cell costs [13] and 15 % of manufacturing costs [14]. Furthermore, the cathode material, which represents 31 % of the cell component costs, is significant for scrap and cost optimization [1].

The quality characteristics of the intermediate products cannot be improved afterward, making it critical to get the production right the first time. Even small variations in production parameters can result in significant changes in product quality, leading to the production of substandard batteries. It has been shown, that small defects in intermediate products, e.g., agglomerates or pinholes in the electrode, affect the performance of the battery cell [15]. For example, agglomerates, as a result of non-homogeneous slurry or deviating slurry feeding rates, lead to lower gravimetric capacities [15]. Moreover, the high susceptibility to particles and contaminants further exacerbates this issue [15].

Due to this susceptible environment quality assurance has to be addressed along the entire process chain to improve the quality of the produced intermediate products and battery cells [16]. As a result, monitoring the quality characteristics and precise adjustment of production parameters are crucial.

3. Data-driven optimization potentials

Addressing the challenges in battery production, data-driven solutions offer a promising potential to optimize the production efficiency, increase quality, and reduce environmental impacts. Particularly, predictive quality, as part of predictive analytics, is a concept that plays a crucial role in enhancing battery production [17].

The large amounts of data generated in the production process pose increasing challenges for companies [18]. The various data sources and data types, such as machine data, process data, and quality characteristics, demands approaches from data analytics, particularly artificial intelligence (AI) and machine learning (ML) [5]. These technologies can help in processing data and extracting valuable patterns, which can support decision-making processes and enhance production efficiency. [19-21] Particularly, machine learning offers the possibility to detect correlations and structures from large data sets.

Data analytics comprises four levels of analytics, which are *Descriptive Analytics*, *Diagnostic Analytics*, *Predictive Analytics*, and *Preventive Analytics* [7, 19].

Descriptive Analytics involves analyzing historical data to identify patterns, trends, and relationships. It helps organizations understand what has happened in the past and how to plan for the future. *Diagnostic Analytics* is focused on understanding the underlying factors that contribute to a particular outcome or event. *Predictive Analytics* analyzes historical and real-time data and make predictions about the future events or trends. Ultimately, *Preventive Analytics* identifies potential problems before they occur. It involves

analyzing data to identify patterns and anomalies that may indicate a future problem. [7, 20]

Predictive Analytics, in particular, aims to use data captured from the production process to make predictions about the future characteristics, such as the product quality, by applying statistical techniques, machine learning, and data mining [22]. Predictive quality, as a part of *Predictive Analytics*, predicts the quality of a (intermediate) product during the production process [7, 18]. The approach involves analyzing data collected from the production process using advanced analytics techniques such as statistical techniques, machine learning, and data mining. This data is used to identify patterns and correlations between various process parameters and the quality of the final product. The applied algorithms can then use these patterns to predict the quality of the final product based on the generated production data.

The challenge in selecting advanced analytics methods is to identify the suitable methods for the specific data and goal of the analysis [17, 23]. Relevant methods are *semantic segmentation*, *decision trees*, *artificial neural networks*, and *support vector machines* [17]. For *semantic segmentation*, a visual object recognition method is used that integrates classifications, statistical methods, and neural networks to assign a class to each pixel of an image [24]. The image can, for example, be generated by a laser scanner. *Decision trees*, on the other hand, are an algorithm that classifies features in order of their relevance [25]. An example of this is a feature vector with b = number of legs and h = body size in meters. *Artificial neural networks*, on the other hand, are used to predict qualitative and quantitative features. They consist of input neurons, an intermediate layer, and output neurons, with weights between the neurons that take values between 0 and 1 [26]. A classic example is an artificial neural network for predicting whether an image is of an apple or a pear. Finally, there is the *support vector machine*, which is an algorithm for classifying features. The separation line is optimized to train the algorithm for classifying new features, and the width of the separating strip is maximized because a wider separating line allows for better classification [27]. On the basis of these data mining methods and the selected data sources and data type, statements about the respective quality of products in production can be made. In combination with the required infrastructure, these methods provide the needed tools for implementing predictive quality.

In battery production, the predictive quality offers high potential as it enables a proactive approach to quality assurance. By predicting the quality of the final battery cell properties during production, potential issues are anticipated and prevented before they occur. The concept allows the adjustment of upstream production steps based on the generated data in preceding processes [28]. This leads to the identification of scrap before the battery cell is fully produced and prevents the generation of production costs, such as energy consumption, in the subsequent process steps [21]. Thus, enables the optimization of production efficiency and sustainability.

In addition, it allows for process optimization by adjusting production parameters once errors or parameter sets impact the final cell quality. For example, if the analysis indicates that a

particular process parameter (e.g., low slurry pump rate) is likely to result in a lower-quality product, the production parameter can be adjusted in real-time to prevent the issue from occurring. This mechanism helps to improve production efficiency and to increase cell quality. Furthermore, it helps to identify the root cause of quality-issues.

The concept of predictive quality has been explored in the literature in single processes or less complex use-cases [18, 29, 30]. However, the implementation of predictive quality in battery production is still a novelty with only few approaches available. FARAJI ET AL implement predictive quality in cathode coating. With a neural network the effects of different coating weights and thicknesses on the battery capacity and internal resistance is modelled. However, with the focus on few intermediate characteristics in one process step a holistic concept including process parameters is missing. [31] LIU ET AL present a similar approach predicting the only intermediate products, such as the mass load, in battery production [32]. THIEDE ET AL propose a more comprehensive concept for predictive quality comprising the process chain in battery production. The concept applies linear regression to predict final cell properties from intermediate products. Nevertheless, the restriction to intermediate products disables the identification of root causes as well as process parameter adjustments. In addition, the modelling is limited to linear regression. [33] A similar approach focusing on the effect of intermediate products on final cell properties has been demonstrated by TURETSKY ET AL [34]. In an additional approach, TURETSKY ET AL detail a prediction model with artificial neural networks deriving the needed intermediate products to achieve certain quality characteristics of the final battery cell. However, the process optimization through predictive quality and the possible identification of scrap during production were not elaborated in detail [35].

Accordingly, a detailing of a holistic concept for predictive quality in battery production is offered.

4. Overarching concept for predictive quality in battery production

Based on the challenges in battery production mentioned before as well as the strong advantages of predictive approaches a comprehensive concept for predictive quality will enhance the production process.

To develop the concept, a fundamental understanding of the interrelationships in battery production is essential. Basically, distinctions can be made along the production process between process and machine parameters, intermediate products and quality characteristics [21, 36]. Process and machine parameters refer to parameters that can be directly adjusted by the production equipment used. This means that process parameters can be directly influenced in the production process. Examples of process parameters are the web speed or the temperature in the dryer. Intermediate products refer to the properties that are determined as a result of the process parameters in a production step and can describe quality characteristics of intermediate products. Intermediate products can thus be set indirectly via the process parameters. Examples are the wet film thickness or the viscosity during coating.

Quality characteristics refer to all quality-relevant properties and features that can be measured on the final product. In the production process they are usually obtained during end-of-line testing of the battery cells. Examples here are the capacity or voltage of the final battery cell. The quality characteristics are a result of the intermediate products and can therefore be indirectly influenced in the production process. [17, 21]

To enable data-driven solutions, such as predictive quality, the correlation of process and product information (intermediate products and quality characteristics) by traceability systems as well as data aggregation in digital twins is needed. [36, 37]

Following these characteristics of the production process for batteries, the application of predictive quality is two-fold. On the one side the characteristics of intermediate products are predicted based on the process parameters for each production process. On the other side predictive quality is applied to predict the quality characteristics (i.e., final cell properties) from the generated data during the production process. [21] The generated quality predictions can subsequently be integrated in feedback mechanisms to enable process optimizations. This allows the direct compensation of quality deviations in the processes preventing the production of lower quality cells or scrap.

Figure 1 highlights the overarching concept for predictive quality in battery production accounting for the distinct parameters and characteristics of the production process.

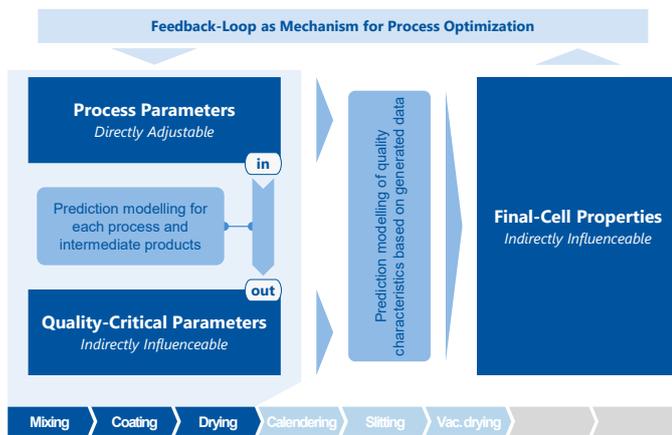


Figure 1: Overarching concept for implementation of predictive quality in battery production

As shown in the figure, the concept includes prediction modeling in two stages for intermediate products as well as quality characteristics. The model for quality prediction of the final cell properties utilizes the used process parameters as well as generated data regarding intermediate products. For this, it is crucial to identify the quality-critical parameters of the intermediate products and to implement the respective measuring methods.

5. Implementing predictive quality in battery production

For the implementation of data analysis projects exist a multitude of frameworks in literature and must be selected based on the requirements and aims of the project. Examples are *SEMMA* (Sample, Explore, Modify, Model, Assess) and

KDD (Knowledge Discovery in Databases) [23, 38]. For the translation of distinct problems into data mining tasks predominantly CRISP-DM and its extension DMME are used in industry. CRISP-DM stands for cross-industry standard process for data mining, which comprises the six phases: *Business understanding, data understanding, data preparation, modeling, evaluation and deployment* [17, 39]. The DMME extension (data mining methodology for engineering applications) addresses the application in the engineering sciences and adds three further phases to account for technical aspects (*technical understanding, technical realization, and technical implementation*). For a successful implementation of the data mining project the consecutive phases shall be followed. [40]

This paper focuses on the technical implementation of predictive quality in the context of battery production. For this, the business value of predictive quality (e.g., in terms of cost benefits through scrap reduction) is not further detailed. Following the framework of DMME, the technical requirements, such as measuring methods, are specified. The technical understanding builds the foundation for the later technical realization and aims to delve into the related expertise and processes. Analyzing the processes in battery production the relevant production parameters must be identified and respective measuring concepts selected. The relevant parameters comprise process parameters, quality-critical parameters from intermediate products, as well as quality characteristics from the final cell. As process parameters and final cell properties can be obtained directly from the production process, the identification of quality-critical parameters in each process step as well as the selection of appropriate measuring methods is needed. For the identification of quality-critical parameters various approaches already exist, which mostly rely on expert knowledge and existing publications [41]. Subsequently, the corresponding measuring methods can be selected. To enable the full potential of predictive quality, the automated data generation should be integrated [42]. For the selection of measuring methods in battery production, this requires the integration of inline measuring methods. Inline measurement is defined as the measurement within the production line and production cycle, i.e., without intervening the production process [43]. This usually complicates the selection of suitable measurement methods for the quality-critical parameters, as there are no inline measurements on a series production scale for some parameters (e.g. porosity). Following the technical realization of the measuring concept, the data understanding, preparation and modeling takes place. In the data understanding and preparation the different data types from the corresponding measurement methods should first be specified and prepared for modelling. Depending on the data type different modelling methods are advantageous, for example, simple values such as the wet coating thickness can be evaluated with decision trees.

Figure 2 shows the technical concept for the implementation of predictive quality for the process step of coating and drying.

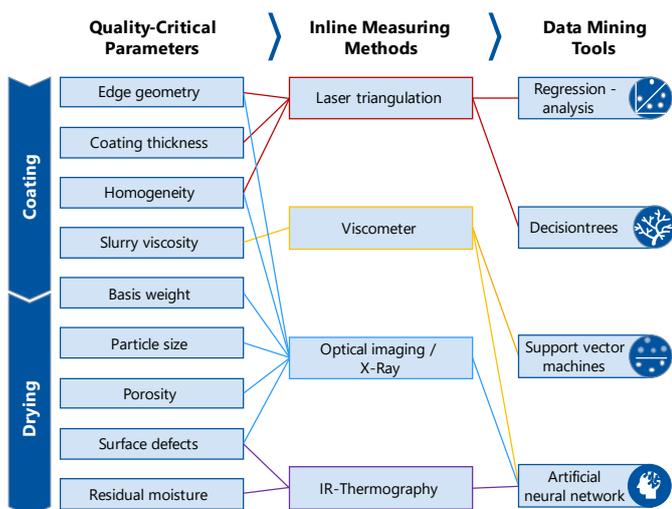


Figure 2: Exemplary implementation of predictive quality in the processes of coating and drying (excerpt).

As highlighted in the figure, various quality-critical parameters exist within coating and drying of the electrodes. Realizing automated data generation, the quality-critical parameters are matched with corresponding inline measurement methods. For example, the geometric values of the coating, such as the coating thickness, can be measured via laser triangulation. Based on the data types of the respective measuring method different data mining models can be applied to evaluate the data and classify the level of quality. In the example, support vector machines can be used to classify the slurry viscosity regarding quality deviations. When using camera-based measuring methods additionally semantic segmentation models should be applied to identify defects in the images. Enabling the prediction of final cell characteristics or intermediate product quality the generated data is used in artificial neural networks.

For predictive quality implementation, first, the set up of the technical infrastructure with the respective measurement methods and data architecture including communication protocols (e.g., OPC UA) and ontologies is needed. This enables the implementation of the selected data mining models. Subsequently, a sufficient data basis must be created through extensive test series. The generated data can then be used to train and validate the quality prediction model. The generation of sufficient data for the deployment of models is often a hindrance in smaller scale productions [21]. Training and validation are essential tasks for the successful implementation of predictive quality for battery production. In the training phase, a large data set of historical data is used to train the prediction model. The model is then validated using a separate dataset to ensure that it can generalize to new data and evaluate the prediction accuracy. [19] Once the model is validated, it can be deployed in the production environment to predict battery quality in real-time. Continuous monitoring and evaluation of the model's performance are critical to ensure that it remains accurate and reliable over time.

6. Conclusion and outlook

The concept of predictive quality offers the potential to solve current challenges in battery production, in particular high scrap rates. The production of lithium-ion batteries comprises a complex and long process chain involving a variety of materials and substantial alterations. Due to the strong correlations between the production process and the product quality, even small variations in parameters result in the production of substandard battery cells. By using data analytics techniques, particularly machine learning, it is possible to predict the quality of the battery cell before production, identify scrap, and create feedback loops to adjust the production process. These benefits lead to more efficient, sustainable, and higher-quality battery production, which is essential for meeting the growing demand for batteries in various industries, particularly in the electric vehicle industry.

This paper presented an overarching concept for implementation of predictive quality in battery production. It was shown how the concept can be implemented by identifying quality-critical parameters and selecting corresponding measuring methods. Based on the automated data generation machine learning methods apply to predict the quality characteristics of the cell. For the process steps coating and drying in electrode manufacturing the technical implementation of predictive quality was shown. After establishing the technical infrastructure on the basis of the concept presented, the quality prediction model can be enabled and deployed in production through comprehensive training and subsequent validation.

For further research, the data acquisition and enablement of quality prediction modelling is in focus. As large amounts of data are required for testing and validation, the utilization of enhancing approaches, such as data enrichment, should be analyzed. Moreover, the evaluation of machine learning models regarding the prediction accuracy of intermediate products and final cell properties, particularly in early process steps, shall be analyzed.

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