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Article

Failure Analysis in Lithium-Ion Battery Production with FMEA-Based Large-Scale Bayesian Network

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Abstract: The production of lithium-ion battery cells is characterized by a high degree of complexity due to numerous cause-effect relationships between process characteristics. Knowledge about the multi-stage production is spread among several experts, rendering tasks such as failure analysis challenging. In this paper, a method is presented, which includes expert knowledge acquisition in production ramp-up by combining Failure Mode and Effects Analysis (FMEA) with a Bayesian Network. We show the effectiveness of this holistic method by building up a large scale, cross-process Bayesian Failure Network in lithium-ion battery production. Using this model, we are able to conduct root cause analyses as well as analyses of failure propagation. The former support operators in identifying root causes once a cell possesses a specific failure by calculating most-probable explanations matched to the individual battery cell data. The latter enable us to analyze propagation of failures and deviations in the production chain and thus provide support for placement of quality gates, leading to a significant reduction in scrap rate. Moreover, it gives an insight into which process steps are key drivers for which final product characteristics.

Keywords: Bayesian Network; Root Cause Analysis; Failure Mode and Effect Analysis; Lithium-Ion Battery Cell; Failure Propagation; Multi-Stage Production; Manufacturing Process; Process Optimization; Scrap Rate

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1. Introduction

Given the necessity of CO_2 reduction in the mobility sector, which is strongly driven by the European Commission's regulations for automotive manufacturers, the shift towards electrification can be observed as one major trend in the industry [1]. Currently, lithium-ion battery (LIB) cells as energy carriers for electric vehicles are one key technology, due to their high energy density and long life cycles [2]. However, there are certain challenges yet to overcome. At the current technological state of the art, LIB cell manufacturers face quality issues, which are reflected in scrap rates of 6 to 12% [3] [4]. This is not only a significant cost factor, but also affects the environmental impact, since LIB production may account for a significant amount of CO_2 emissions during the production of an electric vehicle [5].

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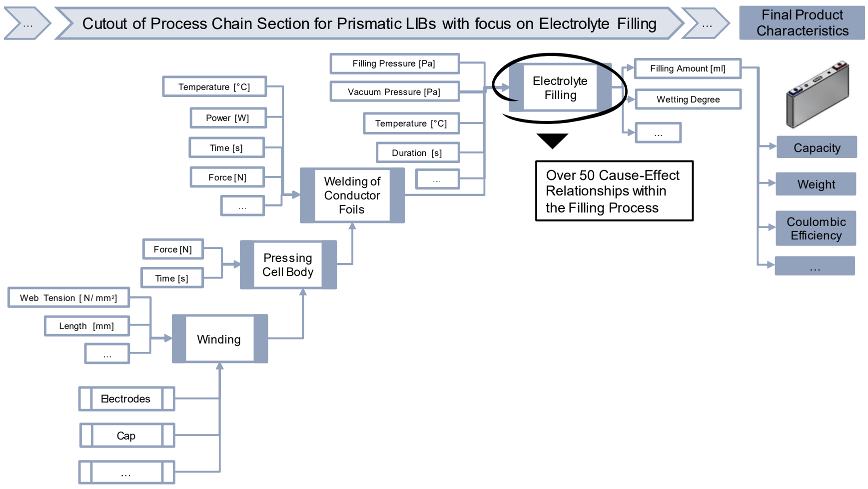

Figure 1. Example of CERs in LIB cell production

According to research, the reason for these scrap rates can be traced back to the high complexity in cell production as a result of many different process steps and a high amount of cause-effect relationships (CERs) between process characteristics [6] [7] [8] [9]. The production of LIB cells involves about 600 process characteristics such as machine parameters and other properties, whose CERs can be depicted as a network consisting of up to 2,100 connections, 75% of which are assumed to be essential for final cell quality [6]. Figure 1 depicts a selection of exemplary CERs in the electrolyte filling process.

Usually a lot of historical production data is available in series production, enabling the application of various data-driven methods upon which failure behavior within a failure network can be analyzed [6] [10]. During prototyping, pilot series and ramp-up, the amount of available production data may still be low, so process corrections due to quality deviations and errors are carried out mostly based on expert knowledge [6] [8]. Considering the complexity, the utilization of expert knowledge for root cause analyses (RCA) gathered by the conduction of quality methods such as Failure Mode and Effect Analysis (FMEA) may easily become strenuous and time-consuming. Furthermore, inconsistencies and contradictions between different ratings can occur during the knowledge acquisition. This is because experts for individual process steps may not able to consider all interactions of their ratings across other process steps. Yet expert knowledge-based quality methods are essential, especially in early-stage production phases [4] [8].

This paper presents an innovative, quality-oriented approach for creating and utilizing a failure network from expert knowledge in the complex process chain of early-stage LIB cell production by combining the benefits of a process FMEA failure network with those of a Bayesian Network. Using a Baysian Network to embody a failure network of the production chain can be beneficial in two ways:

- backward-oriented: provision of algorithmic recommendations during the conduction of an **RCA**, in order to figure out the root cause of a detected failure,
- forward-oriented: failure propagation analysis (**FPA**) within the failure network for the placement of quality gates in the process chain in order to prevent future failures.

It is assumed that incorporation of these two approaches could reduce the time needed to identify root causes of detected failures and, besides that, reduce scrap rates through better understanding of failure propagations and refinement of quality gate implementation.

In section 2, the state of the art and research regarding related topics in traditional quality management is reviewed. Also, current applications of Bayesian Networks in quality assurance are presented. Afterwards, the methods for converting an FMEA into a valid Bayesian Network as well its possibilities for RCA and FPA are presented (section 3). In section 4, the method is applied to build a Bayesian Network based on an expert knowledge-based LIB production failure net. The network is

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then used to gain insights into the production process and to propose promising spots for quality gates. Finally, we summarize our work and derive further research questions (section 5).

2. State of the Art and Research

2.1. Quality Management and Cause-Effect Relationships

A production ramp-up entails special requirements to applied quality methods that consider CERs since data availability is low and parameter specification limits are often not fully defined. Therefore, traditional approaches such as Statistical Process Control, used to optimize processes by means of statistical methods, are not applicable. This limits the selection of applicable quality assurance methods primarily to those that do not rely on quantitative data [8], but rather on expert knowledge. Methods that are based on expert knowledge are henceforth referred to as expert-based methods.

Various expert-based methods designed for the identification and analysis of CERs are available, although only few are suitable for complex manufacturing process chains with a high amount of CERs. Fault Tree Analysis (FTA) and Failure Mode and Effects Analysis (FMEA) are considered to be the most well-established among these [11].

FTA generally follows the principle of building top-down fault trees with numerical information about the failure occurrences, which can be linked to logical gates [12]. The method was designed to analyze malfunctions of subsystems within a larger technical system. Another quality management tool that is often applied to CERs is the Ishikawa Diagram. However, this tool is solely a graphical way to depict CERs without yielding an actual underlying analysis [13].

FMEA comprises an expert-based analysis framework for risk and failure prevention in technical domains with analogies to FTA [14] [12]. FMEA, unlike FTA, also contains qualitative information about the failures, such as correctional measures and failure severity estimations. Different derivatives have emerged from research and industrial projects [15] since the initial introduction of FMEA in 1949, while VDA 4.2 [16] distinguishes between the following main types: Process FMEA (PFMEA) and Design FMEA (DFMEA). DFMEA aims at analyzing the product design itself in terms of quality-critical aspects, while PFMEA was developed to investigate manufacturing or assembly processes and the potential failure CERs involved in these [17] [18]. Other than FMEA or FTA, which are both based on CERs of failures, the method presented in [6] provides a framework for the expert-based assessment of CERs of process characteristics without breaking it down into potential failures of these. Since a process characteristic may have multiple potential failures subordinated to it, the level of details in this method is insufficient for an RCA of failures and deviations in the complex LIB production. RCA is a term in quality management that generally refers to the reactive identification process of a failure's root cause, wherein knowledge that has been gained during application of other quality methods, such as FMEA, can be utilized [19] [20]. The term FPA itself is not as common in industrial standards, however, it may be conducted based on FMEA-derived knowledge in the same way as an RCA.

FTA and FMEA both can be represented as directed acyclic graphs [21] [22]. Therefore, both methods can be utilized as the starting point of a Bayesian Network. However, the qualitative information in FMEA also allows for a preventive failure consequence assessment without requiring much more effort than the creation of the plain failure network with its occurrence rates. This may add further value to the overall achievable process quality.

2.2. Application of Bayesian Networks in relation to RCA and FPA

The cognitive effort of manually conducting an RCA solely based on FMEA failure nets would increase with the complexity of the network and the amount of CERs involved [23]. Various approaches have tried to resolve this shortcoming by making use of different statistical models, each with its own advantages. Extending failure nets to Bayesian Networks has so far shown to be a promising concept [15]. While Bayesian Networks demonstrate a notable amount of robustness against deviations in their parameters [24], they nevertheless lack the direct modeling of uncertainty of expert statements. Other

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potential systems for RCA, such as Credal Networks [25] or Bayesian Models [26], provide a framework to explicitly incorporate uncertainties. This, however, comes at the cost of higher computational complexity especially for large-scale models. Even medium-sized Credal Networks are reported to vastly exceed real-time inference [27]. As the size of the model built in this work is one order of magnitude bigger, Bayesian Networks are preferred due to their scalable inference algorithms.

While an RCA is a reactive, backward-oriented analysis, FPA aims at reducing failures in the future, by analyzing on how individual failure events could propagate and trigger further failure cascades. Also, previous research has shown that Bayesian Networks are helpful means for this analysis [28] [29].

Existing approaches to create Bayesian Networks either rely on quantitative production data [30] [31] or they have been designed specifically for simple process chains, and thus do not involve a proper knowledge acquisition procedure that could be carried out in a reasonable amount of time for complex process chains [32] [33] [34]. Additionally, none of these provide a framework for the continuous improvement of the knowledge base. Still, a Bayesian Network bears intrinsic potential since it can further improve itself and consequently also the FMEA by learning from failures that have occurred after its initial implementation. In the course of the process chain's ongoing growth and maturation, this information can either be collected in the form of error protocols [18] or from user interactions when inquiring the network for the root cause of a present failure [32].

Since LIB cell production consists of interdisciplinary process steps with different process experts in charge, another challenge arises: Mathematical inconsistencies between inter-process expert ratings are bound to occur. In order to ensure that the knowledge acquisition is carried out in a reasonable time while full consistency without contradictions is maintained, experts would need to consider all other ratings that have been made before. Since the human ability to consider multiple interdependencies at a time is limited [23], a validation algorithm is needed to support this process.

2.3. Research Demand

To summarize the current state of research, there is no holistic expert-based method that enables a combined way of creating structured knowledge along a complex manufacturing process chain that can subsequently be used for RCA or FPA. The idea of extending a failure network based on expert ratings to a Bayesian Network, although not new, is highly promising. It would provide an opportunity for probabilistic failure analysis even in cases in which only little or no measurement data is available. Failure information, which is gathered in the course of production advances, can be used to improve the network. Still, existing approaches do not provide sufficient ways for knowledge acquisition in complex processes. Considering hundreds of CERs in a process chain, unstructured knowledge acquisition for uncertain reasoning would be too demanding and could lead to contradicting information. In the following section, a new approach to overcome these shortcomings is presented.

3. Methods

Based on the current state of research, a new method was developed in order to fill the research gap for expert-based failure analysis in complex manufacturing process chains. A failure network from an FMEA in the battery manufacturing process chain is used as a basis to build a Bayesian Network, that can be utilized for RCA and FPA. Due to the advantages that FMEA has over FTA (as described in section 2), an FMEA was chosen to represent the basis for the Bayesian Network.

Leaky Noisy-OR Gates are then used to reduce the number of probabilistic estimates that are needed to create a Bayesian Network and an evolutionary algorithm maintains consistency during knowledge acquisition. After the introduction of the statistical methods, the knowledge acquisition process followed in conducting RCA and FPA is explained in the following sections.

3.1. Bayesian Networks

From a statistical perspective, each failure surveyed in the FMEA is represented by a random variable with binary outcomes – either the failure has occurred or it hasn't. When we denote the number

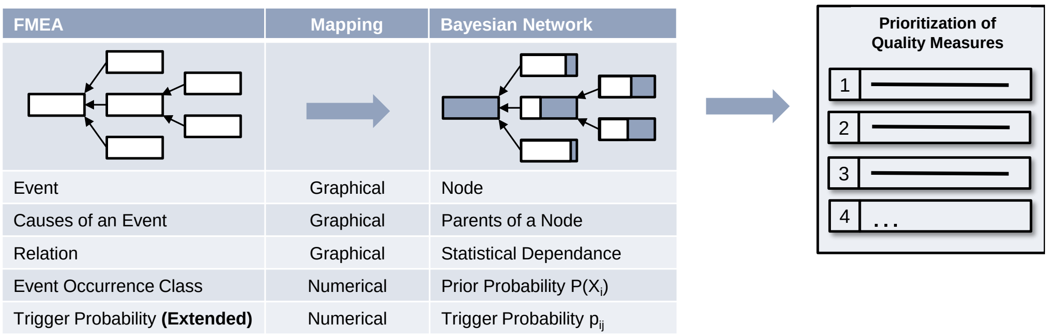

Figure 2. Translation of an FMEA into a Bayesian Network.

of failures in the FMEA as n, we can write all these variables inside a random vector $X = (X_1, \ldots, X_n)$. To represent all influences between the failures, the joint distribution $P(X)$ describing the statistical relations between all variables has to be found. This is a difficult task when many variables are involved, so it requires a way to structure and simplify $P(X)$.

The key idea behind a Bayesian Network is to assume that the probability distribution of each variable depends only on a subset of other variables, its so-called *parents* $\mathrm{Pa}(X_i) = (X_1^{(i)}, \ldots, X_J^{(i)})$. Given these variables, the local distribution $P(X_i \,|\, \mathrm{Pa}(X_i))$ is specified in the form of a conditional probability table. It shows the probability that X_i occurres for each of the combinations of the parents' states. If a variable does not have any parents, it is called a *root node* and solely the probability of X_i occurring is needed, which is referred to as its *prior*. Once all of these local distributions are specified, they can be multiplied to obtain the joint distribution $P(X)$. In terms of graphical representation, the variables stand for nodes in a graph. Arcs exist between a node and its parents, showing their statistical dependency as shown in Figure 2. An in-depth description of Bayesian Networks is found in [35]. The trigger probabilities mentioned in the figure will be explained in section 3.2, but are shown here for the sake of completeness.

Various forms of inference can be made on the completely specified network. Given information about the observed state of some failures, the evidence, the a-posteriori probabilities of all other failures are calculated. One particular use case of these predictions is RCA. This method is applied when a specific failure has occurred and the goal is to identify the cause of this failure, possibly given some more information about other failures. An example of this is given in section 3.6.

The probabilities needed in these inferences can be calculated exactly or, to avoid the runtime-heavy computations, approximated or simulated. Due to the size of our failure network, we decided for simulations using the likelihood weighting algorithm [36]. Roughly speaking, this algorithm randomly generates a certain number of artificial observations from the network. Every failure that has evidence is forced to take its known evidence state. In a last step, the observations are weighted according to the conditional probability of their evidence to gain a non-biased result. The number of generated observations can be increased for more accurate results at the cost of longer computing times. Here, 10^5 observations have shown to be a good compromise.

3.2. Leaky Noisy–OR Gate

As described above, the conditional probability of each variable given an arbitrary combination of its parents' states has to be specified when building a discrete Bayesian Network. However, this number of probabilities rises exponentially in the number of its parents. For example, if a variable has 10 parents, there are $2^{10} = 1024$ different combinations of parent states, and the probability of the variable occurring or not occurring has to be specified for each of these. [37] points out that when asking experts for that many estimates, the quality of the given estimates may decrease. To counteract this, a parametrized distribution can be used to calculate the conditional probability tables from fewer inputs given certain assumptions.

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A common choice for such a distribution is the *Noisy-OR Gate (N-OR)* [38]. It makes it possible to generate the whole conditional probability table by supplying only one probability per variable, thereby reducing the exponential number of parameters to a linear one. The additional parameter is called the *trigger probability* $p_j^{(i)} = P(X_i = 1 \mid X_1^{(i)} = 0, \ldots, X_j^{(i)} = 1, \ldots, X_n^{(i)} = 0)$. It gives the probability that X_i is active given that only one of its parents $X_j^{(i)}$ is active; or in the context of FMEA: The probability that a failure $X_j^{(i)}$ will trigger the failure X_i, given no other known or unknown failures occurred. We use Diez's parameterization of N-OR as the research suggests it provides the best results when surveying trigger probabilities from experts [39].

One of the assumptions of a N-OR is that there are no other causes for X_i than its parents [40], which are the causes surveyed from the process experts. However, it would be naive to assume that there are no other possible causes besides these. Therefore, a *leak variable* $L^{(i)}$ is introduced [41]. It represents all unknown causes of a failure and can be thought of as an additional parent with a trigger probability of 1. To calculate the prior probability of this variable, the gap between the prior probability of X_i surveyed within the FMEA and the marginal probability of X_i given all known causes can be utilized. The exact formula and its proof can be found in the appendix.

3.3. Recommending Consistent Networks

The fact that FMEA surveys prior probabilities even for intermediate failures makes it possible to check for so-called inconsistencies: A failure might happen to be over-explained by its causes, meaning that given the prior and trigger probabilities of the causes, the failure should occur more often than the experts expect. Formally, this means that the marginal probability of a variable given all its parents is higher than its specified prior probability. This occurs due to a mismatch in the variable's prior probability and its parents' prior and trigger probabilities. Note that this comparison is also dependent on the model choice as the marginal probability is calculated using the model. Consequently, the following procedure is only applicable to Bayesian Networks with N-OR assumption and needs to be altered if other models are used.

As will be shown in section 4, there can be several interconnected inconsistencies within a network. To support the expert in resolving these, an algorithm has been developed that searches for a consistent network that is as close to the expert-provided failure network as possible. This suggestion is presented to the expert together with their own FMEA network to help remove potential inconsistencies.

The optimization algorithm will search for consistent prior probabilities and trigger probabilities. However, in FMEA the expert does not directly give prior probabilities, but only occurrence rate classes. Thus, for the prior probabilities, we have to measure the distance of a suggested network to the expert network in the space of these occurrence rate classes. Table 1 shows the probability intervals associated with each occurrence rate class based on the suggestions of [16].

Table 1. Prior probabilities associated with each occurrence rate class

FMEA Occurrence Rate	Probability Interval
1	$[0, \quad 1 \cdot 10^{-6}]$
2	$(1 \cdot 10^{-6}, \quad 50 \cdot 10^{-6}]$
3	$(50 \cdot 10^{-6}, \quad 100 \cdot 10^{-6}]$
4	$(100 \cdot 10^{-6}, \quad 1 \cdot 10^{-3}]$
5	$(1 \cdot 10^{-3}, \quad 2 \cdot 10^{-3}]$
6	$(2 \cdot 10^{-3}, \quad 5 \cdot 10^{-3}]$
7	$(5 \cdot 10^{-3}, \quad 10 \cdot 10^{-3}]$
8	$(10 \cdot 10^{-3}, \quad 20 \cdot 10^{-3}]$
9	$(20 \cdot 10^{-3}, \quad 50 \cdot 10^{-3}]$
10	$(50 \cdot 10^{-3}, \quad 1]$

The problem of searching the closest consistent network can be formulated as a constrained optimization problem with quadratic loss:

$$\text{argmin}_p \left\| \frac{c}{\|c\|} \cdot (q(p) - q_e) \right\|^2$$

constraint: the network generated by p has no inconsistencies.

Here, p is a vector containing the prior and trigger probabilities of a suggested network. As explained above, the vector $q(p)$ contains the corresponding occurrence rate classes and trigger probabilities. q_e contains the expert-given parameters. The vector c contains scalars that represent the costs to change the individual parameters. By utilizing c, different scales between occurrence rates (1 to 10) and trigger probabilities (0 to 1) can be taken into account. Moreover, c could be used to represent the uncertainty of expert ratings. Parameters the expert is not sure about can be changed at lower costs than high-confidence parameters.

The constraint in the above optimization formula can be broken down into several smaller constraints. A network has no inconsistencies if, and only if, the marginal probabilities are smaller than the priors for all variables. This way, the consistency of each variable becomes an individual constraint. Unfortunately, these marginals and their derivatives have no handy functional form, making the optimization infeasible. To handle this issue, the constraints are considered differently: Instead of forcing all suggestions to adhere to all constraints, the number of violated constraints $n_{\text{incon}}(p)$ is added as penalty factor. A hyperparameter α is introduced to balance resolving the highest possible number of inconsistencies and staying close to the expert estimate. Finally, we arrive at the following formula:

$$\text{argmin}_p \left\| \frac{c}{\|c\|} \cdot (q(p) - q_e) \right\|^2 + \alpha \cdot n_{\text{incon}}(p) \; .$$

Due to the rough form of this optimization formula, we apply a genetic algorithm [42] to search for the optimal parameter vector p. Several customizations are made to take advantage of the network structure. When crossing over two suggestions, the parameters are first bundled by the variable they belong to (with trigger probabilities belonging to the variable they trigger) before conducting a uniform cross-over. During mutation, we use a uniform distribution to select a mutation shift for each parameter. For prior probabilities, the span of this distribution equals the width of the probability interval of the corresponding occurrence class in both the negative and the positive directions. Trigger probabilities are not allowed to grow above their expert-given value as increasing a trigger probability beyond this limit can never resolve an existing inconsistency while it always increases the distance to the original expert suggestion, resulting in a worse suggestion. Moreover, the probability of mutation is adapted depending on whether the population's best suggestion has enhanced or become stuck during the previous iteration.

3.4. Building a Bayesian Network out of an FMEA

The whole processes of creating a Bayesian Network from expert knowledge described in the last sections is summarized in this section and visualized in Figure 3. In order to build a Bayesian Network, a proper knowledge base needs to be prepared. This is done by conducting the FMEA in the examined process chain by common FMEA procedure [14]. The procedures may slightly vary according to country or industry, so it is suggested to select one according to the individual requirements of the relevant company. When carrying out the FMEA, experts identify failures throughout the process chain and then try to graphically depict their CERs, which ultimately results in the failure net. After that, experts need to conduct the actual rating of the identified failure CERs in terms of their severity, probability of occurrence and detectability. Along with the occurrence rates, experts are surveyed about the above-mentioned trigger probabilities.

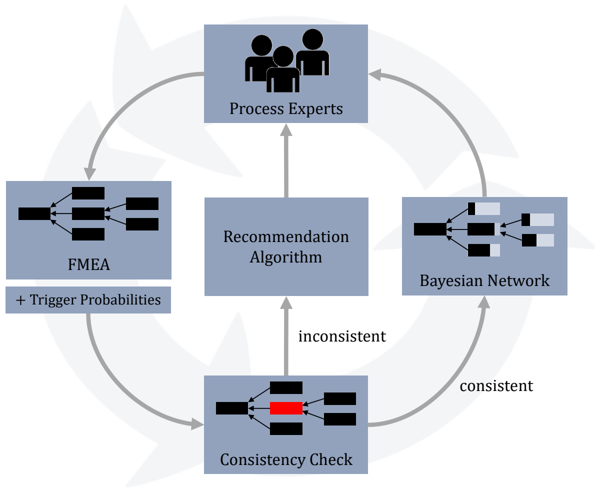

Figure 3. Process for creating a Bayesian Network from expert knowledge

During the FMEA, each process step is analyzed in chronological order. In order to mitigate the risk of inconsistencies, the present failure network with its prior and trigger probabilities is checked for consistency as outlined in section 3.3. Possible lacks in understanding can be revealed by high leak probabilities, and inconsistencies are resolved by the expert with the help of the aforementioned algorithm. Once the FMEA is completed and all trigger probabilities are attached accordingly, the full Bayesian Network is specified, which can be used for inferential inquiries. It can be continuously updated with new failures or other process knowledge.

3.5. Conducting the Failure Propagation Analysis

A Bayesian Network allows to simulate scenarios and interventions by altering some parameters and measuring the influence on the remaining parameters. In the following sections, three different experiments are described that each examine different aspects of the production process, which, as a whole, we refer to as FPA.

3.5.1. Failure Propagation

To analyze the possible propagation of failures, we use the Bayesian Network to simulate the spread of individual failures. For that, we provide the evidence that a specific failure has occurred by setting its probability to 1, and calculate the updated probabilities of all other failures. Most notably, we introduce a new failure called "Cell Rejected" which happens when the produced cell at the end of production fails at least one of 14 final product characteristic tests. The probability of this new failure can be interpreted as the individual cell's scrap probability, or, on production level, as the production's scrap rate. This allows to measure the influence of failures on the scrap rate of the process.

3.5.2. Placement of Quality Gates

Throughout the whole production process of a LIB cell, a cell may experience some minor deviations in process characteristics, which do not necessarily have a severe impact on the final cell. Others, however, may impact the final outcome and thus lead to a defective final cell. Checking for these failures by introducing quality gates at specific points of the production process may thus significantly reduce the scrap rate.

To find out where it is most beneficial to set such gates, we add them to the Bayesian Network as additional nodes behind failure nodes. Their conditional probability table ensures that only cells without the failure will proceed. For each possible location, the influence on the scrap rate was measured, as in section 3.5.1. This method can be applied not only for placing single quality gates, but also for placing

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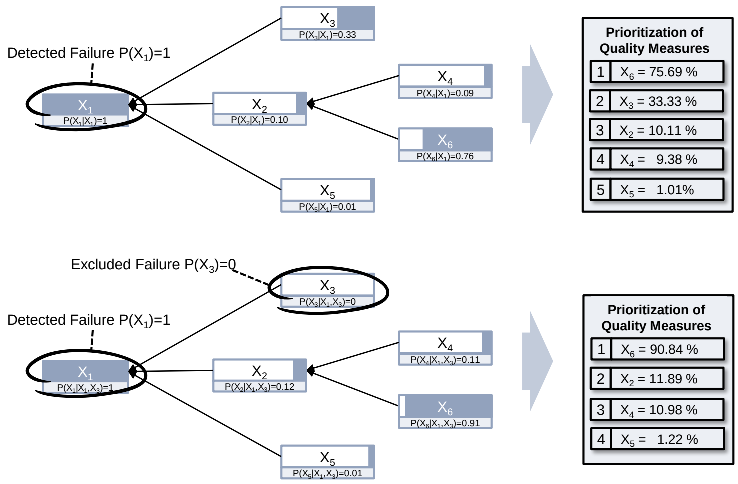

Figure 4. Bayesian Networks with evidence in node X_1 (top) and nodes X_1 and X_3 (bottom).

a whole set of quality gates and measuring their influence. It should be noted that in this analysis, not only the location of the failure in the network, but also its prior have an impact on the reduction in scrap rate.

3.5.3. Process-Wise Influence on Final Product Characteristics

When examining the production on a higher level, it is beneficial to find out which process steps are most responsible for the scrap rate and other final product characteristics and hence have the highest cost-saving potential. To find this out, we simulate a failure-free process step by setting all root causes and leak nodes of that process step to a probability of 0 while all other steps have their usual failure rates. Note that failures in the selected process step can still occur if they are caused by root causes laying in other production steps. Then, as in the previous experiments, we measure the influence of such an ideal process on the scrap rate and several other final product characteristics.

3.6. Conducting the Root Cause Analysis

Once the engineer or expert has observed a failure in the process chain whose root cause could not be instantly determined, an RCA following the described method can be applied. The user can utilize the Bayesian Network to figure out the most likely reasons for the occurrence of the present failure.

A simple example of this inference process is shown in Figure 4. Here, an exemplary failure network with six failures is given. X_1 is the failure that initially occurred – thus, its probability is set to 1 – and whose reason is to be found (top). By using the probabilities returned by the network, experts decide to verify failure X_3. They discover that X_3 did not occur, and feed this back into the network by setting its probability to 0 (bottom). The network now shows that given this additional evidence, X_6 is the most likely reason for X_1 with a probability of occurrence of 90.84%. This interactive process is iterated until the root cause is found. A possible result of such an inference may be that X_6 has occurred and caused X_2 to happen, which in return triggered X_1.

4. Application

The previously described method was applied in the LIB cell prototyping production at BMW Group in Munich, Germany. On the software side, APIS IQ-FMEA-L [43] was the software used to conduct the FMEA. Once exported, the failure network was transmitted to an R [44] script that executed the suggestion algorithm described in section 3.3 using the package GA [45]. During this, 77% of the occurence classes remained unchanged or were changed by at most ± 1 and 73% of all trigger probabilities remained unchanged or were changed by at most ± 0.2, which showed that the network

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was mostly consistent. The final, consistent network was then transformed into a Bayesian Network using the package bnlearn [46] to perform the FPA and RCA.

The Bayesian Network was then used to gather insights into the effects and possible mitigation of failures with the goal of reducing the production's scrap rate. The key findings, which will be further explained in the following sections, are:

- Lithium-ion battery cell production shows a network of highly interlinked CERs across several production steps (section 4.1).
- Failures in early production steps trigger cascades of follow-up failures and thus have a high impact on the final product's scrap rate (section 4.2).
- Quality gates at the right place can stop those cascades and greatly reduce the scrap rate (section 4.3).
- Despite the interconnectedness, specific processes that are key drivers of each final product characteristic can be identified (section 4.4).

Finally, we briefly describe the integration of the Bayesian Network into an interactive dashboard to allow engineers to perform an RCA in section 4.5.

4.1. The Failure Network

The network surveyed through FMEA consists of 432 failures across 20 process steps and 1,098 CERs between them. It is shown in Figure 5 with the color-coded failures according to their associated process steps. This visualizes that failures are highly connected, even across several process steps, thus posing a complex task for failure mitigation. In numbers, 37% of all CERs connect failures across different process steps, and 29.5% of all CERs skip at least one process step, with 8 CERs connecting failures that are 18 steps apart. 219 failures do not have any incoming CER, meaning that they represent root causes. There are, however, failures with up to 32 incoming CERs.

Besides the pure structure of the network, the surveyed occurrence rate classes and trigger probabilities can be analyzed in Figure 6. It can be seen that most failures occur at a rare or medium

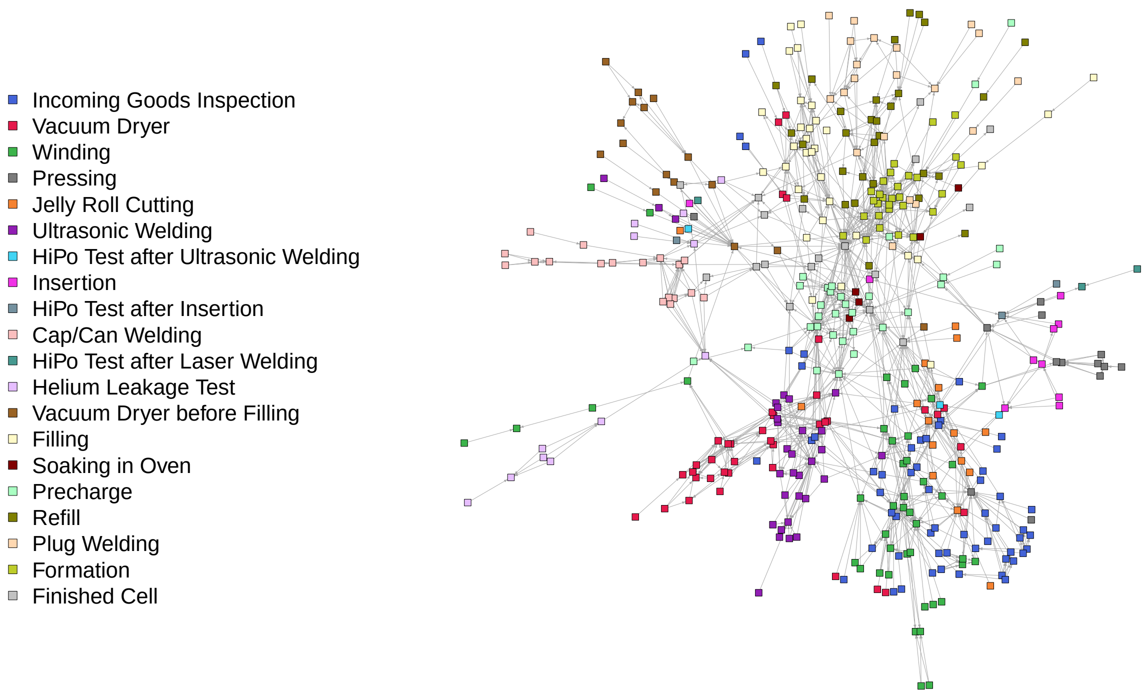

Figure 5. Failure network where each node is a failure color-coded in its corresponding process step (legend of process steps sorted in chronological production process order starting from the top)

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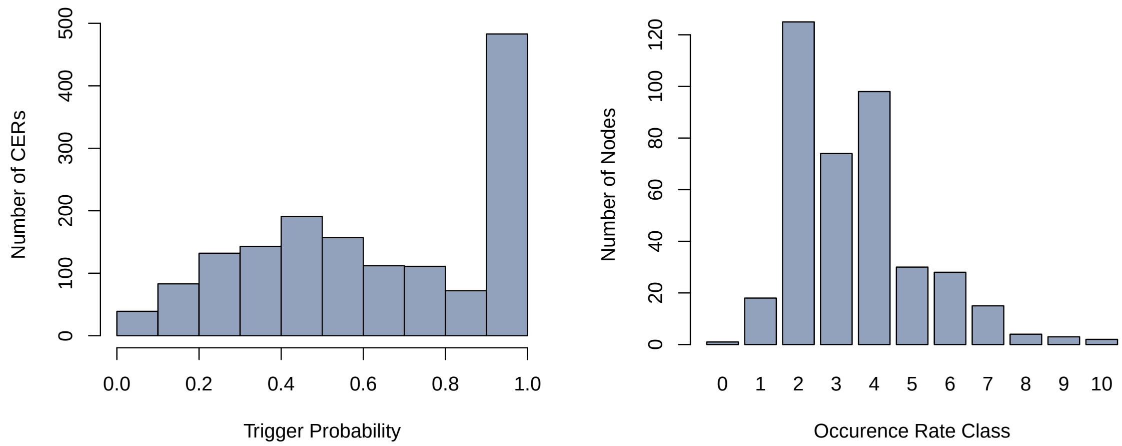

Figure 6. Distributions of surveyed trigger probabilities and occurence rate classes in the network.

frequency, and only a few failures occur often. As for trigger probabilities, the whole spectrum of possible probabilities is used, but nearly every second trigger probability is equal or close to 1. This signifies that a single failure can cause a whole cascade of follow-up failures to spread through the network.

4.2. Failure Propagation

Using the method described in section 3.5.1, we found for 78% of the failures that if they occur, the scrap probability is doubled, and 26% lead to a scrap probability of 90% or higher, thus almost certainly rendering the cell defective. These critical failures do not only occur at the end of production, but also at early process steps. This means that even a failure in the first step (material inspection) can spread through the network, triggering follow-up failures, and lead to an almost certainly defunct cell at the end of production. We call this a failure cascade and analyze how to prevent it in the next sections.

4.3. Quality Gates

Obviously, there is a trade-off between detecting failures in early process steps, which saves more costs and material, and detecting failures in later process steps, where they can be detected more often as they subsume bigger failure cascades. Because of that, we report the top three potential places for quality gates per process step in Table A1 in the appendix. To be precise, we use the term "quality gate" with regard to the observation of the occurrence of one specific failure event". They are ranked by their relative reduction of scrap rate, as explained in section 3.5.2. For example, a bulged cell after refill is relatively simple to detect, and detecting and excluding these cells leads to a 5.56% lower scrap rate compared to the compromised cells going undetected.. Similar failures can be found for each process step, reducing the scrap rate greatly.

To get a first impression of the scale of possible scrap reduction, we iteratively selected the best quality gate per process step and measured how much this set of quality gates reduces the scrap rate (except for the last step as it comprises tests and no more actual production processes). Combined, the 19 selected quality gates lead to a 26.53% lower scrap rate, compared to the case without quality gates. This reduction can be seen on the lower end of what 19 gates can achieve, as the strategy of iteratively selecting the gates is not optimal. The emerging optimization problem can be remedied with the Bayesian Network, but is outside the scope of this paper. However, the accuracy of those predictions is only as accurate as the ratings from the experts they are based on.

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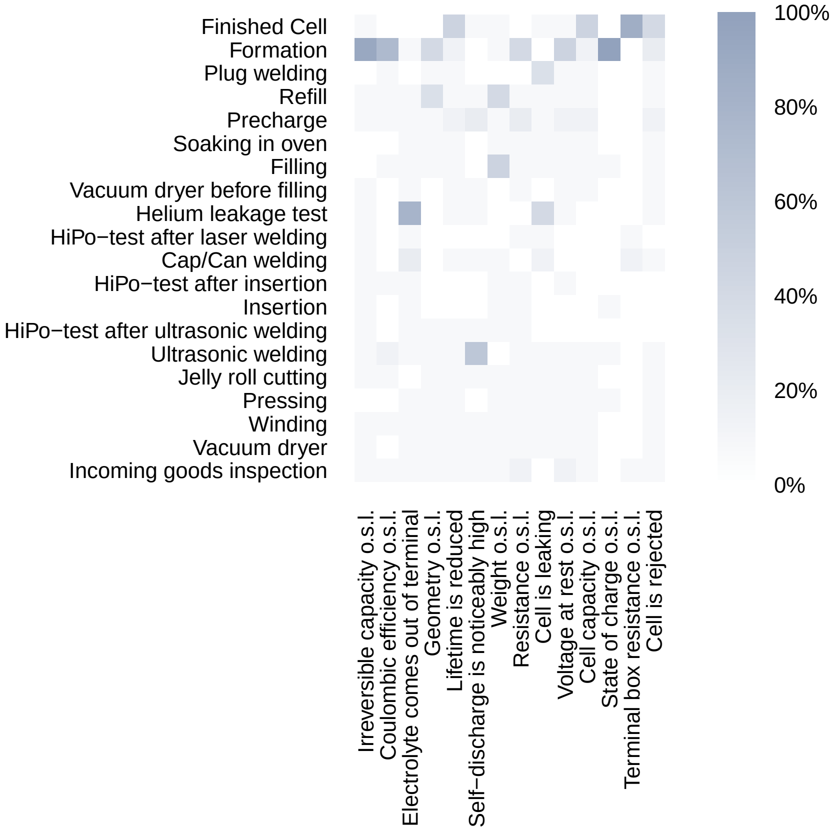

Figure 7. Possible relative reduction of failure rate for several final product characteristics given that a certain process runs failure-free. (o.s.l. = outside the specification limits)

4.4. Simulation of Key Drivers for Final Product Characteristics as an FPA

To analyze the failure network on a higher, process-wise level, we applied the methods described in section 3.5.3. As seen in Figure 7, we found that despite the highly interconnected failure network, some final product characteristics can be traced back to particular production steps as almost their sole drivers. For this, we can look at the columns in Figure 7. For example, a self-discharge in the final cell is mainly caused by the process step of ultrasonic welding, where failures such as scorched electric conductors or cracked electrode foils can occur. When viewing the rows in Figure 7, we can see that improvements in the formation can improve nearly all final product characteristics, making this process a highly interesting candidate for process optimization.

4.5. Implementation and User Interface for RCA

In addition to the forward-oriented approach of an FPA, the Bayesian Network can also be used to support an RCA for produced cells with detected failures, where the exact root cause is not instantly identifiable and thus requires a more specific methodological proceeding. For that purpose, we created a user interface and deployed it on a server as an R-Shiny [47] application.

The user interface for support in an RCA is shown in Figure 8. In this exemplary case, the user initially noticed that the leak rate in the helium leakage test was too high. They confirmed that the cover was not leaky and the RCA suggested to check the welding seam. The user noticed that the welding seam was leaky and the RCA in Figure 8 now shows the possible causes for this, with the seam being burnt during welding the cover ranking highest at an a-posteriori probability of 82.53%.

The user can interact with the tool by clicking either the check mark or the cross in the suggestions to confirm or dismiss a failure. Moreover, they can scan the ID of a cell at hand to fill in information on some possible failures automatically based on its recorded data and passed quality gates. This provides an RCA fitted to the individual cell. As additional information, besides the most likely causes, the

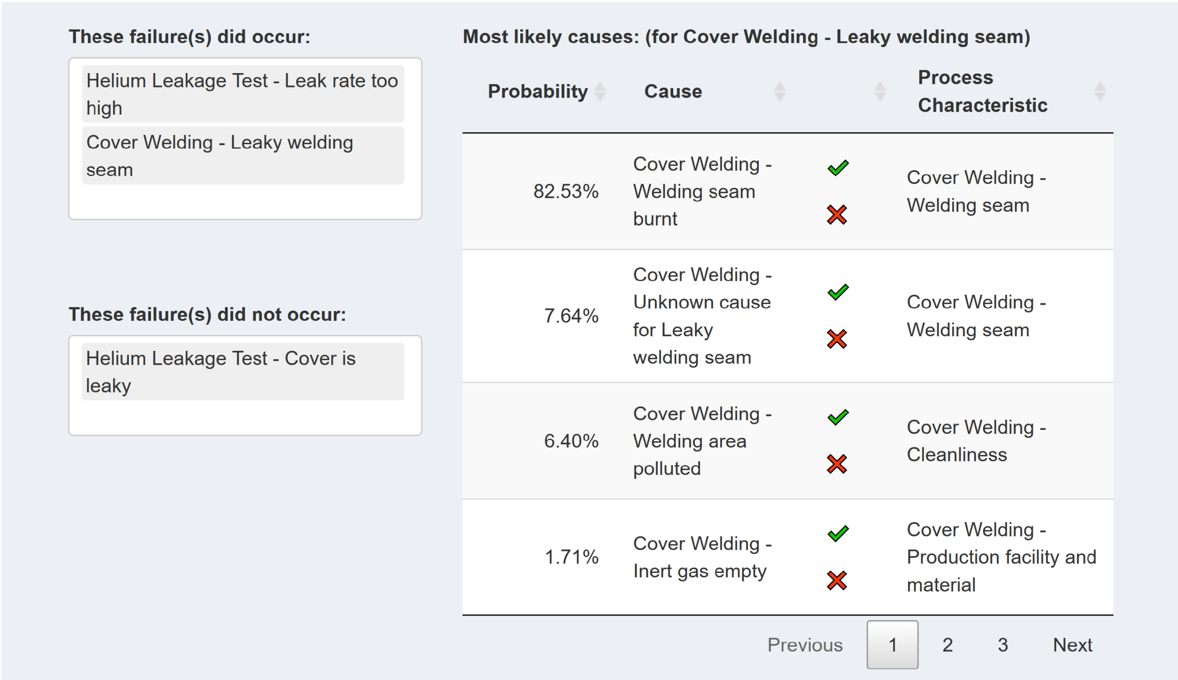

Figure 8. User Interface for RCA.

most likely effects triggered by the given failures can be reviewed for a deeper process understanding. All of the information mentioned is also visualized in an interactive graph similar to that in Figure 4. In future updates, information surveyed in the FMEA on how to detect and rectify individual failures can be shown to provide further assistance.

5. Conclusion and Prospect

This paper presents an FMEA-based method for creating a large-scale knowledge database on possible failures during production from experts, which is transformed into a Bayesian Network under N-OR assumption for backward-oriented RCA and forward-oriented FPA. We used the gathered knowledge to gain insights into where quality improvements and quality gates can lead to a substantial reduction of scrap rate. This method was applied in a multi-stage LIB cell prototype production at BMW Group in Munich, Germany.

We found that battery production features a highly interlinked network of failures and that single failures may propagate and trigger further failure events in the network, which might be an explanation for the high scrap rates in present production. To mitigate these failure chains, we analyzed the most promising locations for quality gates. An exemplary set of just one gate per process step is estimated to reduce the scrap rate by 26.53% compared to process steps without quality gates. Moreover, we used the Bayesian Network to gain a more high-level view on the process, enabling decision makers and process managers to understand which process steps allow for enhancements on which final product characteristics.

Besides the above-mentioned insights, we found it highly beneficial to transform the rather static FMEA results into an interactive tool for RCA. It makes the combined knowledge of several experienced process experts accessible especially to new and less experienced staff and automatically adapts to each individual produced battery cell. Bayesian Networks are a scalable and easily interpretable way to represent knowledge-based failure networks mathematically and to perform inference. Once production data becomes available, the expert-based Bayesian Network can be used as a starting point to be advanced by the data. This makes it a support tool that can accompany the development from early ramp-up phases to mature series production.

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As outlined earlier, the currently used Bayesian Network does not take uncertainties of expert statements into account. Once fast inference algorithms for more complex models like Credal Networks become available, it will be beneficial to include this information. Additionally, as the production is currently still in ramp-up phase, the model built in this work could not yet be tested against observational data. Hence, the above-mentioned insights should only be treated as starting point for further research and process optimization. Once the production yields sufficient data, we intend to quantify the model's performance and use the data to iteratively refine its parameters.

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Abbreviations

The following abbreviations are used in this manuscript:

CER	Cause-Effect Relationships
DFMEA	Design Failure Mode and Effects Analysis
FMEA	Failure Mode and Effects Analysis
FPA	Failure Propagation Analysis
FTA	Fault Tree Analysis
LIB	Lithium-Ion Battery
MDPI	Multidisciplinary Digital Publishing Institute
N-OR	Noisy-OR
o.s.l.	Outside the specification limit
PFMEA	Process FMEA
RCA	Root Cause Analysis

Appendix A. Proof of Leak Probability

Let X_i be an arbitrary node with existing parents $\mathrm{Pa}(X_i)$ and let $P(L^{(i)} = 1)$ be the (unknown) prior probability of the leak variable $L^{(i)}$ of X_i. We can find the value of $P(L^{(i)} = 1)$ that is required to bring the marginal probability of X_i to a predefined value $P(X_i = 0)$ as follows:

$$
\begin{aligned}
P\left(X_i=0\right) &= \sum_{\left(\mathrm{Pa}(X_i),L^{(i)}\right)} P\left(X_i=0 \,|\, \mathrm{Pa}\left(X_i\right), L^{(i)}\right) \cdot P\left(\mathrm{Pa}\left(X_i\right), L^{(i)}\right) \\
&= \sum_{\left(\mathrm{Pa}(X_i),L^{(i)}\right)} P\left(X_i=0 \,|\, \mathrm{Pa}\left(X_i\right), L^{(i)}\right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right) \cdot P\left(L^{(i)}\right) \\
&= \sum_{\left(\mathrm{Pa}(X_i),L^{(i)}=0\right)} P\left(X_i=0 \,|\, \mathrm{Pa}\left(X_i\right), L^{(i)}\right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right) \cdot P\left(L^{(i)}\right) + \\
&\quad \sum_{\left(\mathrm{Pa}(X_i),L^{(i)}=1\right)} P\left(X_i=0 \,|\, \mathrm{Pa}\left(X_i\right), L^{(i)}\right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right) \cdot P\left(L^{(i)}\right) \\
&= \sum_{\mathrm{Pa}(X_i)} \left(\prod_{j=1}^{J} \left(1-p_j^{(i)}\right)^{X_j^{(i)}} \right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right) \cdot (1-1)^0 \cdot P(L^{(i)}=0) + \\
&\quad \sum_{\mathrm{Pa}(X_i)} \left(\prod_{j=1}^{J} \left(1-p_j^{(i)}\right)^{X_j^{(i)}} \right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right) \cdot (1-1)^1 \cdot P(L^{(i)}=1) \\
\Leftrightarrow P(L^{(i)}=1) &= 1 - \frac{P\left(X_i=0\right)}{\sum_{\mathrm{Pa}(X_i)} \left(\prod_{j=1}^{J} \left(1-p_j^{(i)}\right)^{X_j^{(i)}} \right) \cdot P\left(\mathrm{Pa}\left(X_i\right)\right)}
\end{aligned}
$$

Appendix B. Quality Gate Evaluation

Table A1. Estimated relative reduction in scrap rate when a quality gate is introduced to check for the given failures. The table shows the top three failures per process step. (o.s.l. = outside the specification limit)

Process Step	Failure Name	Rel. Reduction
Incoming goods inspection	Wrong material composition of cathode	0.507%
	Insufficient adhesion	0.447%
	Wrong material composition of anode	0.369%
Vacuum dryer	Excessive moisture in the cathode	0.222%
	Excessive moisture in the anode	0.219%
	Anode coil diameter is too large	0.202%
Winding	Coating defects	0.905%
	Telescoped jelly roll	0.475%
	Detaching solvent	0.450%
Pressing	Thickness o.s.l.	1.355%
	Force increase o.s.l.	0.254%
	Pressing time o.s.l.	0.239%
Jelly roll cutting	Cutting burr is too large	0.613%
	Film layers are torn	0.306%
	Particles adhere to cut edge	0.229%
Ultrasonic welding	Anode height o.s.l.	2.079%
	Cathode height o.s.l.	2.016%
	Particles on surface	1.110%

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Process Step	Failure Name	Rel. Reduction
HiPo test after ultrasonic wielding	Testing voltage is set incorrectly	0.147%
	Dew point o.s.l.	0.077%
	Isolation resistance is too low	0.053%
Insertion	Isolation foil has holes	0.134%
	Insertion cannot be carried out	0.115%
	Insertion power o.s.l.	0.102%
HiPo test after inseration	Isolation resistance is too low	0.099%
	Dew point o.s.l.	0.063%
	Testing voltage is set incorrectly	0.028%
Cap/Can welding	Point of welding is scorched	0.611%
	Weld seam is leaking	0.469%
	Laser is stopped during welding process	0.145%
HiPo test after laser welding	Dew point is below specification limit	0.135%
	Testing voltage is set incorrectly	0.070%
	Isolation resistance is too low	0.053%
Helium density test	Leakage rate is too high	2.624%
	Burst membrane is leaking	1.553%
	Given criterium of leaking rate for o.k./not o.k. does not correspond to the applied helium overpressure	0.371%
Vacuum dryer before filling	Remaining moisture is too high	1.411%
	Temperature o.s.l.	0.292%
	Retention time o.s.l.	0.208%
Filling	Volume of dosage o.s.l.s	0.982%
	Weight o.s.l.	0.614%
	Bursting membrane is damaged	0.506%
Soaking in oven	Electrolyte was not soaked up sufficiently	1.184%
	Retention time o.s.l.	0.199%
	Cell is bulged after soaking	0.064%
Precharge	Loading capacity o.s.l.	2.740%
	Voltage at rest is decreasing continuously	1.648%
	Inner resistance o.s.l.	1.234%
Refill	Cell is too bulged	5.563%
	Weight o.s.l.	0.952%
	Dosing volume o.s.l.	0.672%
Plug welding	Point of welding is leaking	1.349%
	Area of welding seam is polluted	0.744%
	Welding seam resistance is too low	0.659%
Formation	Cell is too bulged	10.644%
	Capacity o.s.l.	5.405%
	Execution is interrupted	2.886%
Finished cell	Lithium plating appears	25.182%
	Lifetime is reduced	21.211%
	Cell capacity o.s.l.	17.945%

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