

Cross-domain reliability analysis from individual components to the entire system during development using the example of a lithium-ion battery cell

Entwicklungsbegleitende domänenübergreifende Zuverlässigkeitsanalyse von Einzelkomponenten bis hin zum Gesamtsystem am Beispiel einer Lithium-Ionen-Batteriezelle

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Abstract

Using the development of a lithium-ion cell as an example, an analysis of the reliability of individual components is carried out during development. For example, the effect of newly developed anode materials on the reliability of the entire system can be determined. If data are available, the effect of design specifications on (system) reliability can be calculated quantitatively down to the battery module. With the help of Bayesian Networks, the logical linking of the failure modes with quantitative failure rates from the individual component to the battery cell is represented. For the optimization process of individual components, the effect in the battery module can thus be calculated directly. This is particularly necessary because different developers are usually involved in the various sub-domains for the individual components of a lithium-ion cell. This makes it possible to keep the focus on the reliability of the overall system across company boundaries. Particularly regarding of the current increased development of battery cells without the use of critical raw materials such as cobalt, it is important to evaluate new alternatives directly in the development process, not only in terms of performance, but also in terms of reliability.

1. Introduction and motivation

Further product developments of complex technical systems are particularly challenging in terms of system reliability and safety. This is especially more likely when fundamental changes are made in different domains. It becomes even more complex when different developers implement changes in different parts or subcomponents of the technical system in the early phase of the design process. Often there are dependencies between different domains with significant effects on reliability. Keeping track of these different changes is challenging in terms of different areas such as mechanics, electrics, chemistry and different developers of the companies involved. Using the example of the development of a cobalt-free lithium-ion battery

in the EU project COBRA (COBalt-free Batteries for FutuRe Automotive Applications), a method to address the challenges mentioned before is demonstrated. Additionally, the description and tracking of quantitative reliability data over the design process of different generations of the cell and battery pack is shown. The project calls for a holistic approach to address the many challenges associated with the development of reliable lithium ion batteries. With the method, the effects of individual changes on the overall system can be represented and calculated, which supports the development of a novel, reliable, cobalt-free lithium-ion battery.

2. Introduction to Bayesian Networks

Bayesian Networks belong to the family of probabilistic graphical models and are directed acyclic graphs. They can visualize knowledge about an uncertain domain [1]. Each node of the graph represents a random variable with at least two discrete states. Each edge represents dependencies between the related random variables. These conditional dependencies can be estimated using numerical and statistical methods. In order to express conditional probabilities of a single variable in dependence on others, Bayesian networks use Conditional Probability Tables (CPT). Bayesian Networks are used, for example, in the field of artificial intelligence [2]. A number of solving algorithms for the exact or approximate solution of BN have been developed throughout the recent decades such as the variable elimination (VE) algorithm [1].

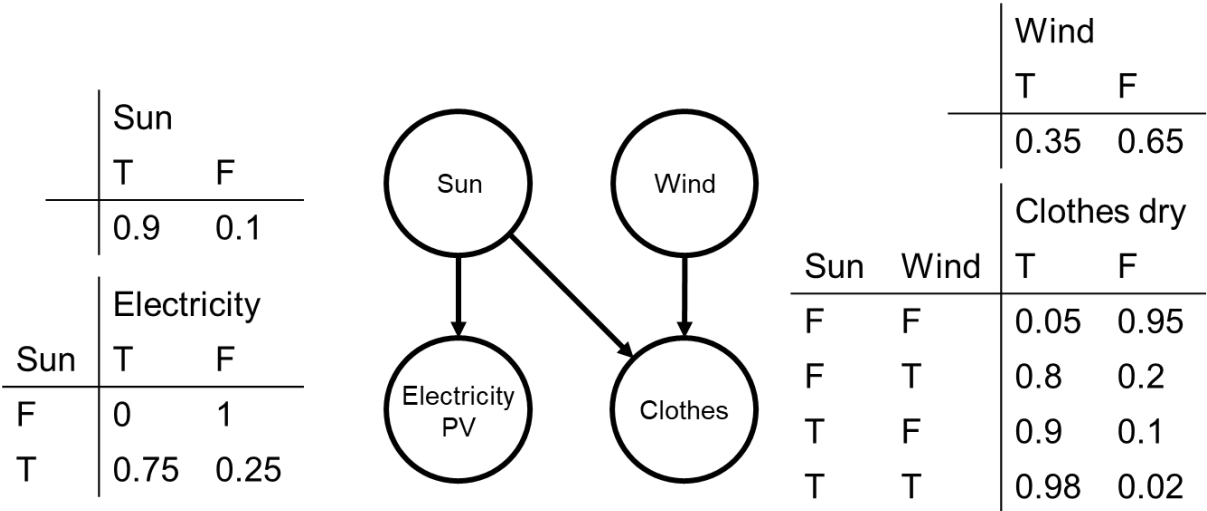


Figure 1: Bayesian Network with conditional probability tables

With the help of a fictitious graph, which can be seen in figure 1, the principle of Bayesian Networks is explained. CPTs are used here to express conditional probabilities (true = T, false = F) and its associated probabilities (0 – 1) of a discrete state. Whether the sun is shining or not and whether there is wind are mutually exclusive states of the random variables. These represent evidences which occur with a certain probability during a fictitious time span of three

hours. In the example case wet clothes that have been hung out to dry will dry during this period if the sun is shining on the clothes and it is windy. The sun is to hit on the photovoltaic system from the right angle to convert enough sunlight into electricity in order to charge a scooter battery, for example. This outcome is independent of whether there is wind.

3. Introduction of safety methods for technical systems

To determine the reliability of a system in a qualitative analytical way, various methods are available, such as Failure Mode and Effects Analysis (FMEA), Fault Tree Analysis (FTA) and event sequence analysis [3]. To assess reliability, this can be done either with a bottom up or top down approach. Bottom up means that this is carried out through the hierarchy levels starting with the components or subcomponents up to the overall system. For this, failure modes for sub-components are being determined and their effects and consequences concluded with respect to the group of integrated sub-components. In the top-down approach, the failure search in the system is carried out starting with the system to identify possible causes in the lower hierarchical levels. FMEA is a systematic bottom-up method to determine all potential failure modes, failure effects and failure causes for components or (sub-)systems. The risk is determined and recommended actions for optimisation are defined. For each failure mode, it is qualitatively determined how likely the occurrence of a failure mode is, how severe the consequences are and how likely the cause is detected [3]. Based on the FMEA, the failure modes, mechanisms and effects analysis (FMMEA) was developed, which follows a physics of failure approach. The FMMEA approach can be used to gain a better understanding of the failure mechanisms and physics-of-failure that lead to failure modes [4].

FTA is an analytical top-down technique that defines an unintended state of the system (top level event) that predominantly is critical from a reliability or safety perspective. The system is then analysed in the context of the environment and operation to determine the ways in which this top level event can occur. With the help of a graphical model represented by the FTA, various parallel and sequential fault combinations that lead to the top level event can be identified and displayed. To evaluate FTAs, minimal cut sets (MCS) are usually created, i.e. the smallest possible combination of basic events that trigger the top level event. In particular, MCSs triggered by only one fault or event are to be avoided. Fault trees can also be evaluated quantitatively by specifying the probabilities for the occurrence of basic events for each MCS and adding up the probabilities of the individual MCSs that lead to the top level event [5]. The results of the calculations with MCS can deviate from the exact probabilities and must therefore be viewed with caution or generated with other evaluation algorithms [6].

Since FMEA does not allow quantitative evaluation, FTA does not allow a coherent holistic representation of the system Kaiser and Rauschenbach [7], [8] proposed a concept for

quantitative FMEA called probFMEA which can be modeled and solved based on Bayesian Networks. Bayesian Networks are used for this purpose, which provide the algebraic basis to allow the quantitative assessment of reliability.

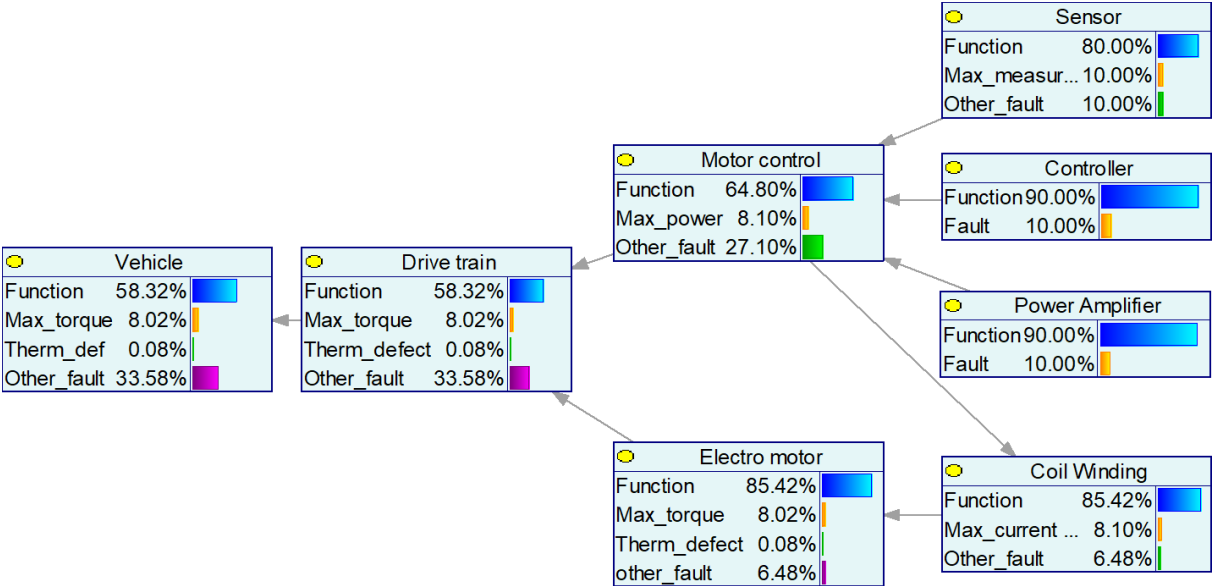


Figure 2: Example of a cascade fault as a conditionally independent consequential effect modelled with Bayesian Networks [8]

An exemplary failure network of an electric vehicle based on Bayesian Networks is shown in Figure 2. If a malfunction occurs in a component, e.g. in a sensor, the condition is propagated to the next higher hierarchy level (motor control) and then to the drive system and finally to the vehicle level. A cascading fault was realized as a conditionally independent consequential effect [8] in this example.



Figure 3: Quality and significance of the data depending on the available data

The significance of the Bayesian Network depends on the quality of the available data for the failure modes, the logical cause-effect relationships, and the corresponding failure probabilities. At the beginning of the network creation, when not enough failure probabilities are available, a rough estimation is made to understand the cause-effect relationships. As the development of a product progresses, more data gradually becomes available, as can be seen in figure 3, and the network becomes more significant.

4. Design of lithium-ion batteries he cell upwards

A conventional lithium-ion cell consists of a lithium-based cathode, a carbon-based anode, electrolytes and a separator, as shown in figure 4. Usually, the cathode material is bonded to an aluminium foil and the anode material to a copper foil, both of which act as current collectors. The electrolyte consists of soluble salts, acids or other bases in the liquid and dry polymer. A piece of porous polymer serves as a separator and is located between the anode and cathode. The separator is immersed in the electrolyte and serves as prevention against a short circuit between the two electrodes. During operation, lithium-ions undergo a cycle of intercalation and deintercalation and move as charge carriers through the electrolyte in the internal circuit. The intercalation of the lithium-ions into the anode needs an external energy and the deintercalation happens spontaneously. During this process of the lithium-ions, redox reactions occur at the electrodes, which generate electrons that form a current through the external circuit. The migration of the lithium-ions in the internal circuit and the migration of the electrons in the external circuit enables the battery to operate [9].

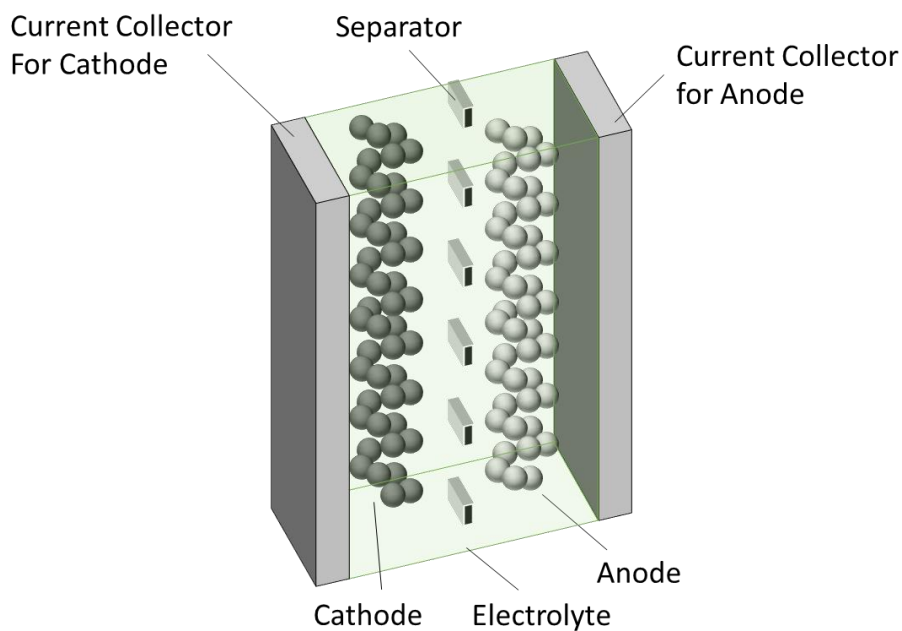


Figure 4: Basic structure of a lithium-ion battery cell based on [12]

Since individual cells cannot provide the necessary power for applications in electrified vehicles, for example, several cells are electrically and mechanically interconnected to form modules. Modules usually contain electrical and thermal sensors and interfaces. The mechanical and electrical assembly of several modules is called a battery pack, which usually contains hardware and software for thermal and electrical control. By combining the modules into a battery pack, the necessary power and energy for electric vehicles can be provided. In

the automotive context, battery packs are embedded in the existing crash safety structure and communicate with the vehicle electronics to operate the cells with the intended operating parameters in terms of safety and lifetime [10].

In [11], [12] the most important degradation mechanisms in lithium-ion battery cells that occur during operation and exposure to environmental conditions were summarized.

While some failure modes can be attributed to wear during operation, certain failure modes are due to overstress. These can be attributed to operation outside the defined operating conditions as e.g. deep discharge or environmental conditions as e.g. mechanical stress. Hendricks [12] has divided the observed effects caused by the failure modes of the ten cell components into thirteen types. Some of these imply a reduction in performance (e.g. reduced cell capacity) while others have safety-critical consequences such as a thermal runaway. To avoid premature degradation and catastrophic failure, constant monitoring and control of the lithium-ion battery is essential. Without proper control of operating conditions, the battery system is prone to failures that can cause explosions, fire, toxic gas emissions or other negative consequences for both humans and the environment.

5. Application of the probabilistic FMEA

Based on a FMMEA of a lithium-ion battery cell from Hendricks [12] and the probFMEA approach from Rauschenbach [8] a Bayesian Network with logical connections between the failure modes of battery components and the observed effects on cell level is created with the software GeNIe[®] Modeler from BayesFusion which is shown in figure 5. Instead of each battery component being a separate node with its associated failure modes as shown in figure 2, each failure mode has been given its own node to facilitate the graph handling. Based on this Bayesian Network, a qualitative and quantitative analysis of the reliability of a lithium-ion cell can thus be carried out. To limit the dimensions of the created CPTs, additional nodes are inserted which have no effect on the calculated results. Instead, these serve for a systematic bundling of inferences related with specific functional consequences, such as reduction of capacity or power or increased diffusion resistance. In order to increase the manageability and clarity of the graphs, the components with its failure modes are grouped into sub models.

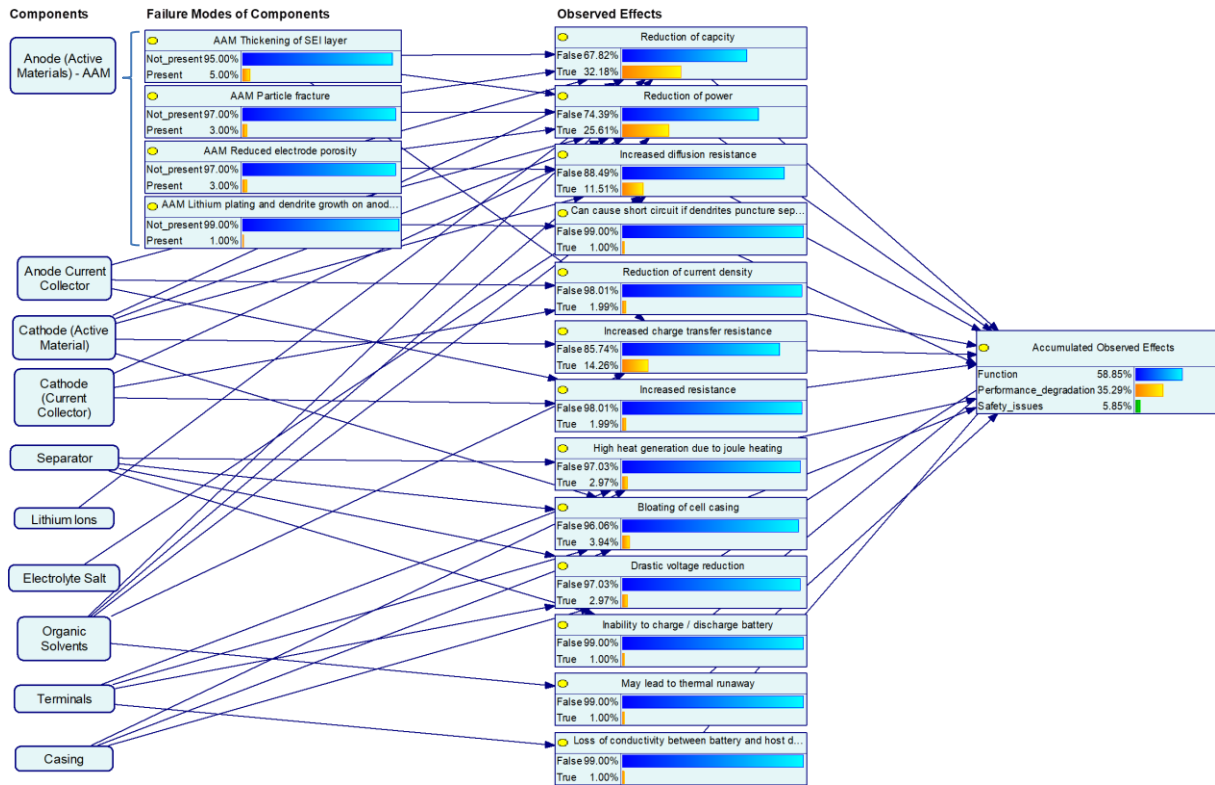


Figure 5: Bayesian Network with failure modes of a lithium-ion cell with fictitious failure probabilities

Since the technology of lithium-ion batteries is not entirely new, data from existing systems or from literature can be obtained to refine the Bayesian Network. In the next step, the developers of the components and materials can make initial statements about how high the failure probabilities are and which cause-effect relationships exist. In order to validate and verify the generated failure networks and failure probabilities, component tests, integration tests and system tests are to be carried out. As the number of tests increases, the Bayesian Network can be updated in a recursive manner with more accurate data. Due to the lack of precise data for failure probabilities the shown percentages are derived from Hendricks FMMEA based on reliability testing, battery disassembly and failure analysis with its division into high/moderate/low likelihood of failure occurrence in the battery lifetime [12]. Failures of the identified components can lead to various observed effects on cell level which are grouped into several categories based on their impact on the cell (function / performance degradation / safety issues). Section 4 explained how the use of sensors and control of operating conditions in the BMS of a battery pack can result in less catastrophic consequences than those depicted in the Bayesian network of a single cell shown in figure 5. As the failure probabilities depend heavily on the use cases and load profiles as well as the environment types in which the battery is being operated, these parameters need to be determined for a more accurate result.

Because of the nature of the Bayesian Networks, the presented methodology can be extended across several hierarchical levels of a battery system from component level up to the battery pack level as outlined in figure 6. In the context of electric driving, this can be continued up to the vehicle level.

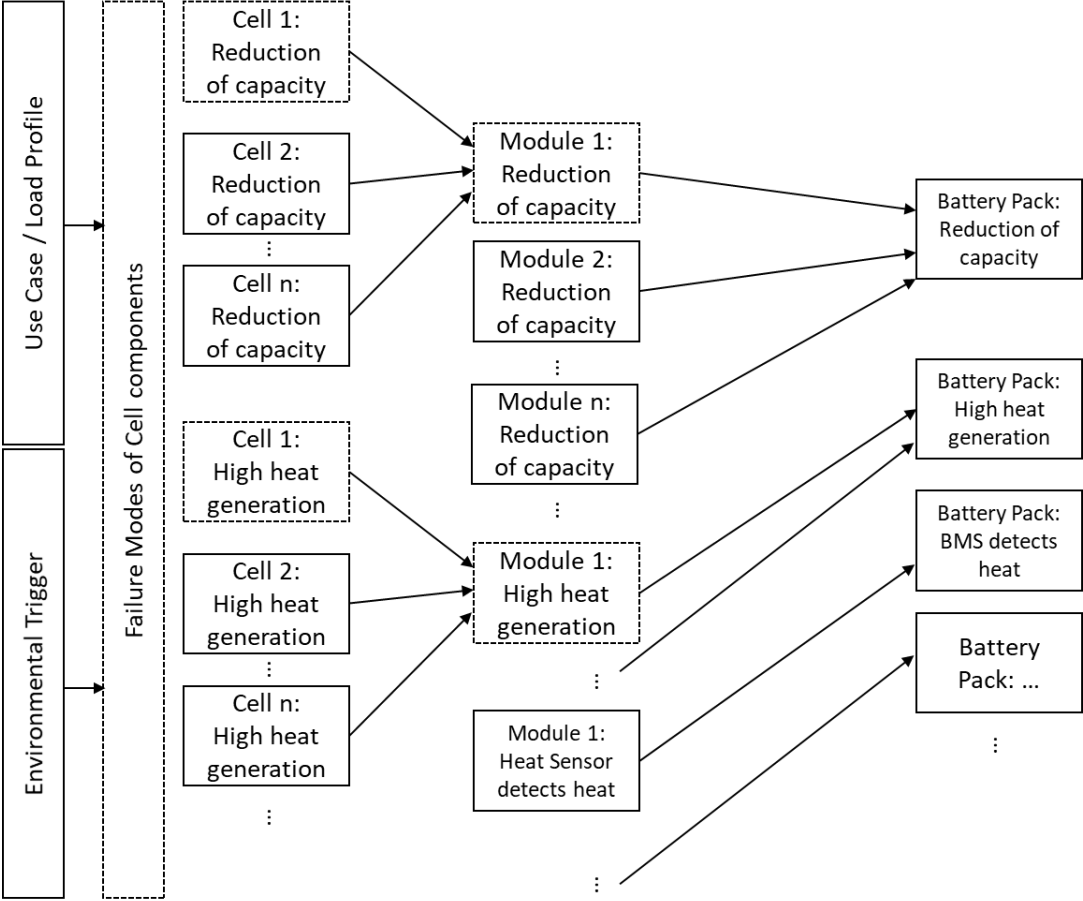


Figure 6: Outline - Extension of the Bayesian Network with observed effects on module and battery pack level

The blocks highlighted with dotted lines were discussed in detail in the previous section. The related failure modes per cell can be collected and accumulated for each failure symptom addressed per module and subsequently per battery pack to estimate the failure probabilities of the whole battery system. The propagation of failures in individual cell components can thus be modelled up to the top level. If sensors are installed at module or battery pack level to detect faults, this can also be taken into account in the model. Depending on the use case and load profile, e.g. operating the battery close to the design limit can have a negative impact on the reliability and safety of the individual components. This can be taken into calculation of the Bayesian Network in addition to the influence of environmental conditions such as extremely low ambient temperature.

Figure 7 shows how the development of new materials or components can affect the probabilities of the observed effects under the assumption that all components not shown do not change its failure modes and probabilities. In this fictitious example, the impacts of a newly developed anode material and a new organic solvent on the observed cell-level effects are modelled. An important capability of modelling with Bayesian Networks is the fact that comparisons between different model generations can be made visually and numerically to measure the progress of the project. It can happen that on the one hand the performance is increased due to the use of new components. But on the other hand the probability of a critical condition (e.g. high heat generation) may increase at the same time. If this condition can be avoided through the smart use of sensors and risk mitigation by a battery management system (BMS), the net result is a gain in performance without a loss in safety. This methodology makes it possible to address different areas such as mechanics, electrics, chemistry and the different developers of the companies involved and quantify the safety and reliability of newly developed products. When used in the early concept phase, this tool can help make design decisions that affect reliability and safety, contributing to the development of a safer product. At the points where the presented methodology identifies vulnerabilities, developers can implement failsafe and mitigation measures that would prevent an undesirable state of the battery cell.

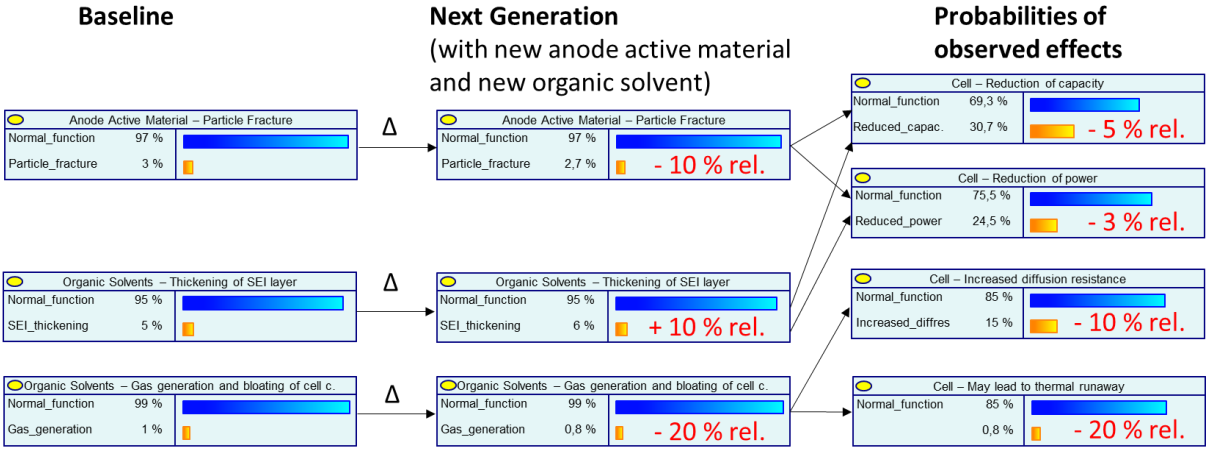


Figure 7: Comparison of two battery material generations and the observed effects

Besides the incremental change of probabilities, the failure modes can also be set to completely true or not true, in order to determine the possible consequences. A major advantage of Bayesian Networks is their use for reversed evaluation from specific observed symptoms to the likelihood of possible causes, termed as back propagation.

Table 1 (left): Most likely Failure Modes with its associated fictitious probabilities when *Increased Diffusion Resistance* (IDR) is present - Table 2 (right): Observed effects that occur simultaneously as an impact of IDR

Component	Potential Failure Mode	P [%]	Observed Effect	P [%]
Organic Solvents	Gas generation and bloating of cell casing	43.45	Increased diffusion resistance	100
Anode (Active Material)	Reduced electrode porosity	26.07	Reduction of capacity	64.94
Cathode (Active Material)	Reduced electrode porosity	23.07	Reduction of power	61.54
Organic Solvents	Thickening of solid electrolyte interphase layer	8.69	Increased charge transfer resistance	14.26
			May lead to thermal runaway	8.69

In this fictitious example, increased diffusion resistance was assumed to be true ($P = 100\%$). Based on the fault network presented at the beginning, the most probable failure modes can be determined sorted according to their occurrence probabilities, which can be seen in table 1. Since a large part of the observed effects do not occur alone, side effects can be identified, sorted by probability of occurrence, as shown in table 2 to have a better understanding of the mechanisms.

6. Summary and outlook

In this work, a methodology was presented to analyse the reliability and safety of a lithium-ion battery cell. Logical relationships between failure modes and observed effects were created in a Bayesian Network. With this approach, it is possible to qualitatively and quantitatively assess as well as visually display the reliability and safety of further developments across different domains during product development. Depending on the availability of data, incremental changes to individual components and their effects on the cell can thus be determined. In the COBRA project, the approach will be pursued to reveal weaknesses and to monitor the development of a safe and reliable cobalt-free battery across different battery generations. For this step, the Bayesian Network is extended to module and battery pack level, including fail safe mechanisms and risk mitigation strategies. Using selected components as examples, a comparison between a state of the art battery containing cobalt and a cobalt-free battery will be yielded. In order to be able to make more accurate assessments, data from laboratory tests

and validation tests of the cell, modules and also the battery pack will be used. The methodology shown here is not limited to the development process of batteries, but is applicable to a wide range of complex technical systems, such as autonomous driving or systems with fuel cells.



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