Available online at www.sciencedirect.com

ScienceDirect

Procedia Manufacturing 43 (2020) 720–727

Procedia MANUFACTURING

www.elsevier.com/locate/procedia

17th Global Conference on Sustainable Manufacturing

Multi-Criteria Optimization in the Production of Lithium-Ion Batteries

Thomas Kornas[a,c]*, Dominik Wittmann[b], Rüdiger Daub[a], Oliver Meyer[b], Claus Weihs[b], Sebastian Thiede[c], Christoph Herrmann[c]

[a]*BMW Group, Technology Development, Prototyping Battery Cell, Munich, Germany*
[b]*Chair of Computational Statistics, Technische Universität Dortmund*
[c]*Chair of Sustainable Manufacturing and Life Cycle Engineering, Institute of Machine Tools and Production Technology (IWF), Technische Universität Braunschweig*

Abstract

Lithium-ion-batteries (LIBs) play a key role in determining the environmental impacts of future mobility technologies. In particular, the production of LIBs has a strong environmental impact as it is characterized by high scrap rates. In addition to existing expert-based approaches for the identification of quality drivers in production, a trend towards data-driven methods is discernible. Nevertheless, most approaches show shortcomings in the involvement of multi-criteria optimization. Therefore, this paper uses desirability functions to jointly optimize several quality parameters. Validation was conducted based on the data of an assembly line for prismatic LIBs.

Keywords: Lithium-Ion Battery, Desirability Functions, Quality Management, Multi-Criteria Optimization

1. Introduction

Transportation of people and goods is continuously increasing, causing significant CO_2 emissions [1]. In 2013, 17.3% of the overall energy-related greenhouse gas emissions were caused by road transportation [2]. Driven by the European Commission's call to reduce vehicle fleet emissions to 95 g CO_2/km by 2020, the electrification of vehicles represents one of the most visible trends in the automotive industry [3]. Compared to internal combustion engine

* Corresponding author. Tel.: +49-151-601-79830; fax: +49-89-382-70-10021.
E-mail address: Thomas.Kornas@bmw.de

10.1016/j.promfg.2020.02.113

vehicles, electrified vehicles offer high powertrain efficiency and are marked by a lower CO_2 footprint [4]. Assuming an average European electricity mix and a vehicle lifetime of 150.000 km, the use of an electrified vehicle has a global warming potential (GWP) of approx. 20% compared to an internal combustion engine vehicle [4].

Due to their high energy density, long life cycle and shelf life, lithium-ion batteries (LIBs) play a decisive role in the successful electrification of vehicles [5]. The production still shows enormous potential for enhancing sustainability, which is not least reflected in a significantly high scrap rate of 5-12% of series production [6,7]. Moreover, LIBs are responsible for 50% of CO_2 emissions during the production of an electric car [8]. On the one hand, the high share of CO_2 emissions can be attributed to the ambient production conditions, such as a required dew point of up to -60 °C [9]. On the other hand, the high waste heat generated in the drying process of the coated electrodes is a main energy driver [10]. In addition to the high energy requirements in production, the embedded materials in LIBs must also be considered for a holistic view on sustainability. Nickel-manganese-cobalt (NMC) oxides are nowadays considered the state-of-the-art materials for the positive electrode, whereas cobalt in particular is regarded as a valuable since it represents a scarce resource [10].

The high scrap rate, as a key factor in determining sustainability, is caused by a unique form of complexity in the production of LIBs and is regarded as a major topic of current scientific publications [7,9,11–15]. The complexity is caused by an interdisciplinarity within the production, in which process, electrical and manufacturing engineering are brought together. Moreover, the production is characterized by a large number of process steps, and each individual process step is defined by numerous influencing variables, such as material properties, process parameters, or quality characteristics. Consequently, the process chain for LIBs entails an interlinked set of root causes [11]. Thereby, processes and products as well as their interactions are not well understood compared to more established sectors [12]. The majority of the root causes are regarded as relevant in terms of LIB quality. However, the quality is not only defined by one but several properties, such as the capacity, weight and coulombic efficiency, which can potentially lead to conflicting goals [12,16]. The increasing demand for battery cells in the automotive sector will lead to an expansion of manufacturing capacities [17]. In order to reduce the scrap rate and thus the environmental impact, a holistic approach to optimizing the quality of LIBs is necessary. One the one hand, the approach must be suitable for complex productions with interlinked root causes. On the other hand, a multi-criteria analysis has to be included in order to jointly optimize several quality properties and thus meet the customers' requirements.

This paper is structured as follows: The second chapter summarizes the state of the art and current research regarding the specified requirements for LIB production. Subsequently, in chapter three, the mathematical concept of desirability functions as well as a comprehensive framework for quality management in LIB production are presented. Chapter four describes the application and evaluation of the presented framework at the BMW Group's production line for prismatic LIBs.

2. State of The Art and Research

A large number of methods are available, which aim for quality optimization of complex systems. Two fundamental requirements can be derived from the introduction, which represent the major evaluation criteria of the state of the art and research:

- Suitability for complex process chains with interlinked root causes
- Capability of multi-criteria optimization for several quality properties

Generally, quality methods for the analysis of root causes can be subdivided into expert- and data-based approaches [11]. The Failure Mode and Effects Analysis (FMEA) can be regarded as an established expert-based method for the systematic, experience-based recording of failures, risks and consequences. As explained in [11], the FMEA is not applicable for complex process chains with a large number of root causes. Therefore, Westermeier [18] presents a qualitative approach to investigate factors influencing the quality of LIBs based on multiple domain matrices. However, the method presented by Westermeier is not capable of performing a multi-criteria analysis.

Current developments in the context of Industry 4.0 have led to the availability of large amounts of data and thus to the application of data mining, which describes the general process of knowledge discovery from databases [19]. Recent publications show a tendency to apply data-driven methods for quality improvement, such as demonstrated in

[20] and [21]. Facing the challenges of complexity in the manufacturing of LIBs, Schnell et al. [22] use a data mining approach in order to improve quality. The publication was based on the Cross Industry Standard Process for Data Mining (CRISP-DM). Although good modeling results were achieved, a multi-criteria optimization of several target properties was neglected, as only the capacity of a LIB was analyzed. Thiede et al. [12] recently published a further approach for a data-driven analysis and improvement in the production of LIBs. The author's framework aims to predict the quality of a LIB on the basis of influencing variables. In contrast to Schnell et al., several target properties were analyzed. Within the presented framework, the decision support module represents an essential element, in which visual analytics (e.g. heat maps or correlation networks) are made available to the domain experts. Furthermore, p-values and regression coefficients for different target features are plotted in the form of a portfolio to support the domain process experts in a further improvement. However, their approach does not provide a prediction for optimal values of influential variables regarding the overall product quality. Their focus lies on the identification of factors that influence the product quality.

As previously stated, the optimum values of influencing variables, such as material properties or process parameters, might be distinct for different quality properties (e.g. weight, capacity or coulombic efficiency). Considering the fact that the capacity is directly proportional to the integrated electrode material and thus to the weight of a battery cell, it is often not possible to improve one quality feature without deteriorating others. A suitable way to consider multiple quality properties was presented by Meyer et al. [15]. The authors' approach is based on desirability indices and allows to combine a merged score of several quality properties under specification restrictions. Nevertheless, the applicability of the method has not been provided yet for a whole process chain with a large number of root causes, as Meyer et al. only focused on the optimization of a single process step. Moreover, the data for their analysis was provided by conducting a design of experiments (DOE). Hence, it was generated under isolated conditions. The distinguishing characteristic of real-world settings is that no prior definition of the sample space is conducted, which might lead to considerable challenges in the data pre-processing [23, 24].

Further approaches for multi-criteria optimization were discussed in [30]. It can be deduced that desirability functions are suitable for various problems (maximization, minimization, targeting). In addition, they are understandable and provide a good linkage to domain experts.

A reduction of the scrap rate in LIB production has a major environmental impact. It can be summarized that recent publications showed a tendency to use data-driven methods to handle complexity in production. In particular, Thiede et al. successfully showed that data mining can be applied to a quality-related assessment as well as to improve planning and control. Nevertheless, there is a significant gap to identify the optimum values of influencing variables for different quality properties. Desirability indices can address these challenges and are therefore discussed in the following chapter. Additionally, a framework is presented showing how desirability indices can be implemented in an overall quality system.

3. Method

Desirability functions offer the possibility of multi-criteria analysis. For their calculation, it is essential to include expert knowledge, e.g. the weight of quality properties of a LIB or specification limits of process parameters. Thus, the expert knowledge can serve as input for a quality management system. It would be conceivable to use specification limits for statistical process control (SPC). In the following, an overview of desirability functions is provided. Subsequently, a framework is presented in which expert knowledge, SPC and desirability functions can be combined.

3.1. Desirability Indices

This chapter presents the basic idea of desirability functions as a method for multi-criteria analysis. The simultaneous optimization of several quality parameters entails a number of challenges. On the one hand, the parameters are measured applying different measuring scales and physical units. On the other, it must be assumed that the optima of the quality parameters differ in the values of the input variables and cannot be achieved simultaneously. In the worst case, the optimization even runs in opposite directions. The desirability indices provide a solution for both problems. At the same time, they offer the possibility to integrate expert knowledge. As described by Steuer [25], in the first step, each quality parameter is transformed by means of an individually defined desirability function to a unit-less scale. The desirability scale should be limited to the value range from 0 to 1. A higher desirability stands for a "better" value of the parameter. In the following, three common desirability functions and their advantages are presented (Fig. 1). The desirability functions described here are only a selection.

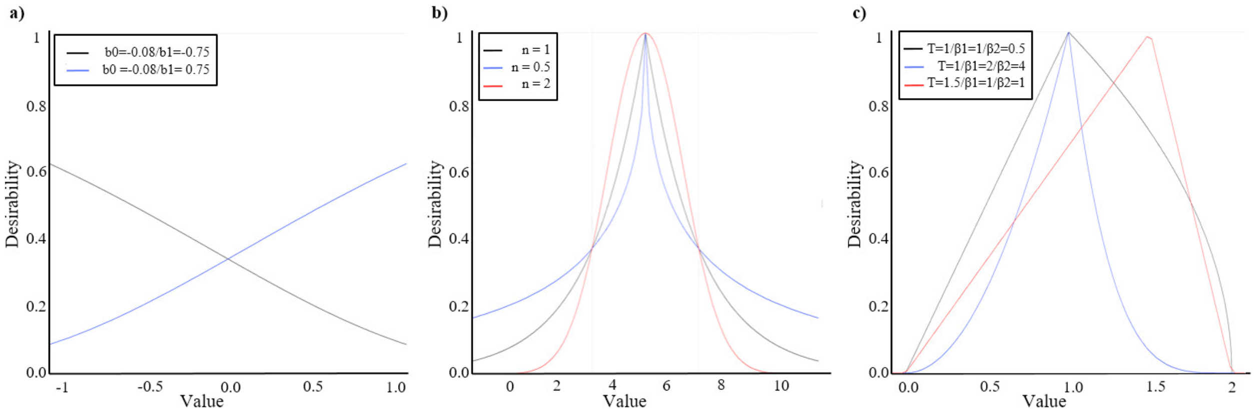

Fig. 1.Desirability functions: (a) one-sided Harrington; (b) two-sided Harrington; (c) Derringer-Suich

One-sided Harrington

The one-sided desirability function d_1 for a quality parameter Y introduced by Harrington [26] is defined as follows:

$$d_1(Y') = e^{-e^{-Y'}}, \qquad \text{with } Y' = b_0 + b_1 Y. \tag{1}$$

This function sets neither hard limits above which the desirability are 0 or 1, nor other outstanding values. Instead, the function is monotonous over the entire value range. This makes the one-sided Harrington function suitable for parameters that only become "better" or "worse" with increasing values.

Two-sided Harrington

Harrington [26] also introduced the following two-sided desirability function d_2:

$$d_2(Y') = e^{-|Y'|^n}, \qquad 0 < \text{n} < \infty, \text{ with } Y' = \frac{2Y-(USL+LSL)}{USL-LSL}. \tag{2}$$

Here, LSL/USL designate the lower/upper specification limits that must be specified by experts. Outside the specification limits, the function assumes small values of desirability, but does not make a hard cut. The function runs symmetrically around the center of the specification range at which the desirability equals 1.

Derringer-Suich

Derringer and Suich [27] proposed the following more flexible desirability function:

$$d_3(Y) = \begin{cases} 0, & \text{for} \quad Y < LSL \\ \left(\frac{Y-LSL}{T-LSL}\right)^{\beta_1}, & \text{for} \quad LSL \le Y \le T \\ \left(\frac{USL-Y}{USL-T}\right)^{\beta_2}, & \text{for} \quad T < Y \le USL \\ 0, & \text{for} \quad USL < Y. \end{cases} \tag{3}$$

Outside the specification limits, this function falls directly to 0. By setting a target value and two shape parameters, a lot of input is required from experts, but it also offers a lot of scope for design.

For each quality parameter, individual statistical models are created using linear regression. The variable selection for the models is made from all input variables of the previous process steps as well as from the process steps of the quality parameters themselves. As an example in the production for LIBs, the amount of electrode material and electrolyte can be considered as input variables. The total weight of a LIB could represent a quality parameter which is influenced by these input variables.

Predictions of the quality parameters can be calculated based on linear regression, which are then transformed with the desirability functions. These transformed values of the predictions of the various quality parameters can be converted into a desirability index using a weighted average [25]. The weights of the weighted mean value can be used to control how important the quality parameters are to be in comparison. The individual models themselves are optimized in such a way that the overall desirability index is maximized. Since the quality parameters are transformed to the same value range via the desirability functions, cross-process comparisons can take place. Individual process steps can also be evaluated and a type of variable importance can be specified.

3.2. Framework

The framework presented in Fig. 2, in which the desirability functions are embedded, is based on the CRISP-DM process model [28]. It contains some modifications in order to implement the desirability functions, especially as, in contrast to the common CRISP-DM, these integrate expert knowledge. The main differences are found in data preparation and modeling.

Once the prepared data is available, the first descriptive statistics can be created to gain a deeper understanding of the data. These statistics include simple indicators as well as visualizations. These can help the process experts to define specifications, target values, desirability functions including their parameters as well as extreme values. The experts may then have to specify weightings of the quality parameters for the calculation of the overall desirability index. In case of a large number of quality parameters, a pairwise comparison can be applied by domain process experts in order to conduct a scientific study for the weighting of quality parameters. Subsequently, statistical modeling and optimization is performed as described above.

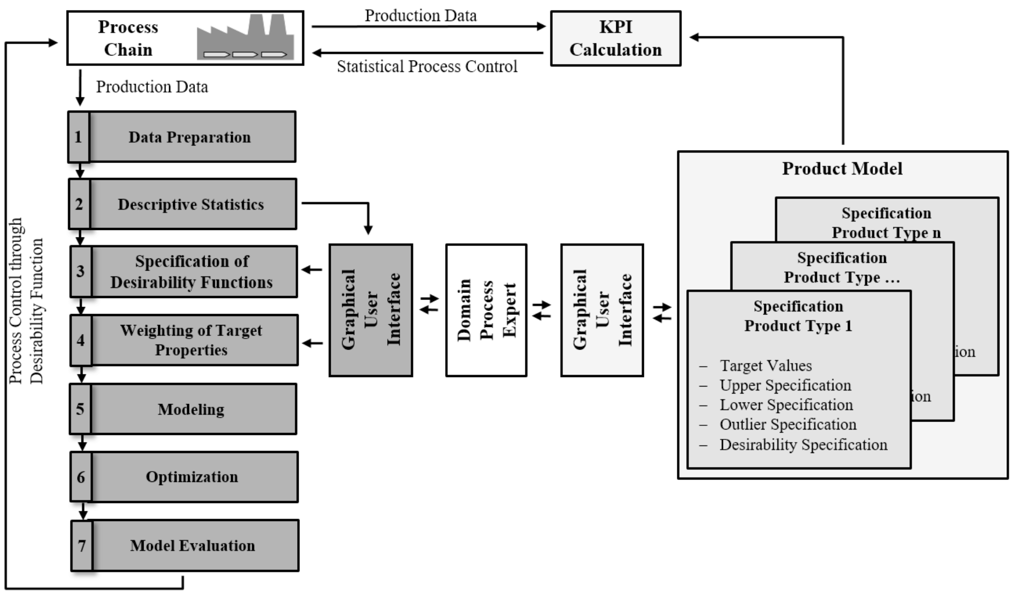

Fig. 2. Framework for implementing desirability functions in an overall quality management system.

Particularly in the prototype phase, but also in series production, different product types may exist. The expert knowledge of each product type should therefore be stored in a structured database, which is described as product model in Fig. 2. Via graphical user interfaces, the product model and the visualizations of the descriptive statistics can thus be used to easily compare the characteristics of different types of LIBs. A further advantage lies in tying the product model to a KPI calculation. In the first stage of a KPI calculation, the specification limits (USL and LSL) of each feature can be compared to their measured value in order to conduct a SPC. Furthermore, it would be conceivable to use multivariate process capability indices for a root cause analysis, as demonstrated in [11].

4. Application and Evaluation

An application and validation of the framework was conducted using the data of the prototype assembly line for prismatic LIBs at the BMW Group in Munich. The production consists of 16 consecutive process steps, which are depicted in Fig. 3. For a detailed description of each process step, reference is made to Korthauer [10]. For the application, a total of 400 LIBs with a specific cell type (NMC622) were analyzed. A total of 167 parameters, including process parameters, intermediate product characteristics from analyses and tests, as well environmental influences, were measured.

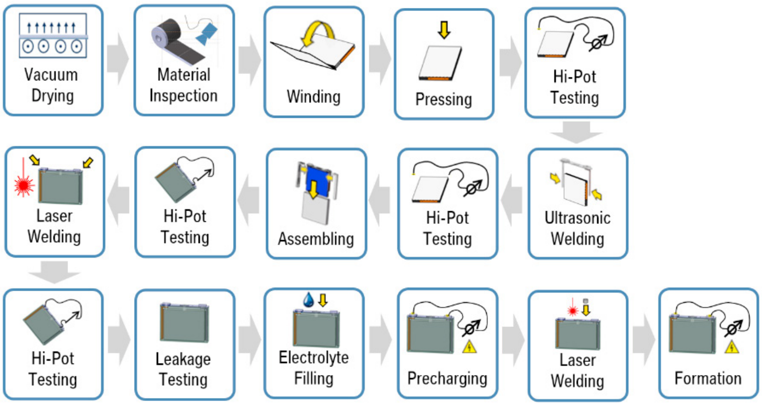

Fig. 3. Process chain of the assembly line for prismatic LIB cells.

A multi-criteria optimization with the help of desirability functions was realized for two of the quality parameters, battery capacity and battery weight. As depicted in Fig. 4, for the battery capacity, a one-sided Harrington function was used, as this quality parameter gets better with increasing value. A Derringer-Suich function was used as desirability function for the battery weight. In a first step, the target values as well as specification limits (LSL/USL) were defined by process experts. The target value of the battery weight corresponds to the desirability of "1". As shown, the process expert considers a battery weight above the target value to be more critical than below.

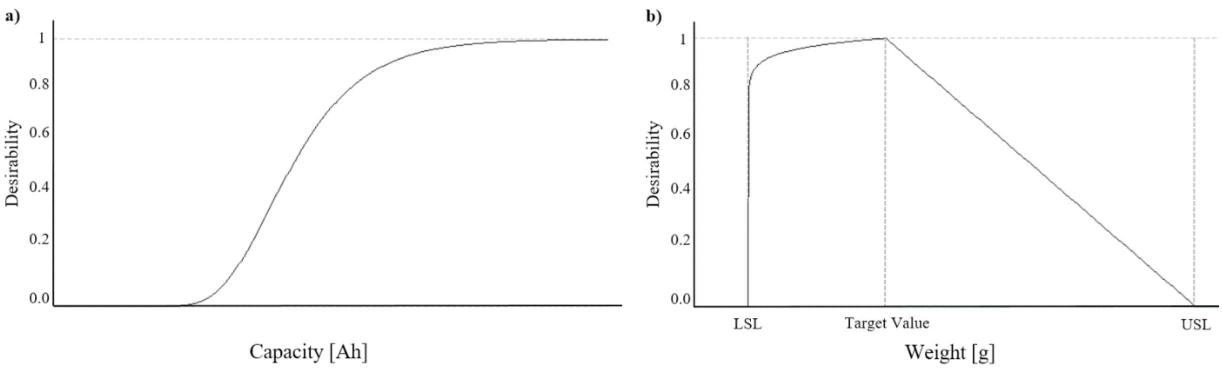

Fig. 4. Expert-evaluated desirability functions; (a) One-sided Harrington for the capacity of a LIB; (b) Derringer-Suich for the weight of a LIB.

In the use case study, three optimizations with different weightings of the quality parameters for the desirability index were calculated. The first optimization was used as a reference and therefore applied a uniform weighting of the quality parameters. The other two optimizations weighted the quality parameters at a ratio of 1:2, once with respect to the battery capacity and once with respect to the battery weight. The concrete values of the input variables that lead to the optimum values of the quality parameters are not provided. Instead, the results from the optimizations with the 1:2 weightings are given as deviation from the values of the reference optimization, as depicted in Table 1. In this way, the table shows the percentage by which the parameter changes to the original setting.

The results of the case study can be interpreted as follows: The influencing variables are attributed to the electrolyte filling and the winding process. The electrolyte filling pressure influences the wetting degree that effects both the capacity and weight [29]. Furthermore, it is notable that an increase in the electrolyte amount leads to a reduction in weight. However, this apparent contradiction can be explained as follows: The prismatic battery cell has a defined volume due to its hard case. Since the electrolyte density is lower than the density of the electrode, a weight reduction can primary be achieved by decreasing the electrode length.

Table 1. Selection of influencing variables and their percentage change with weighting on battery capacity and battery weight.

Process step	Influencing variables	Deviation of the influencing variables with weighting on the battery capacity	Deviation of the influencing variables with weighting on the battery weight.
Electrolyte filling	Filling pressure 1	- 3.68 %	+ 2.6 %
Electrolyte filling	Filling pressure 2	+ 1.61 %	- 0.93 %
Winding	Electrode length	+ 0.42 %	- 0.42 %
Electrolyte filling	Electrolyte amount	- 0.41 %	+ 0.41 %
Winding	Winding speed	+ 0.12 %	- 0.01 %

The described example demonstrates the necessity of a multi-criteria analysis in the production of LIBs. The reduction in scrap rate using desirability functions is not provided in this paper, as this requires a statistical significant number of LIBs to be produced. However, the case study provides the optimized variables for such a production.

5. Conclusion and Outlook

Uncertainties caused by a unique form of complexity are the main driver for high scrap rates in the production of LIBs. The presented framework demonstrates a novel approach that can be applied to field data in order to improve quality management in complex production chains. Desirability functions represent a fundamental component of the framework, allowing for a multi-criteria analysis. Moreover, the framework combines expert knowledge with established quality management methods, such as statistical process control.

Several conclusions can be drawn: Using data from the assembly line for prismatic LIBs, desirability functions have been successfully applied in complex production systems, revealing how input variables affect different quality parameters. In the next step, the optimal values of the input variables, which were calculated based on the model are to be applied in production to provide evidence of a reduced scrap rate. Moreover, validation was conducted for only one product type in LIB production. However, a large amount of quality-relevant variables relate to the electrode production, which was not considered in this use case study. The electrode production inevitably leads to an increase in complexity in modeling and must therefore be investigated in future research with regard to the scrap rate.

References

[1] J. Léonardi, M. Baumgartner, CO2 efficiency in road freight transportation: Status quo, measures and potential, Transportation Research Part D: Transport and Environment 9 (2004) 451–464.
[2] D. Birol, CO2 Emissions from Fuel Combustion 2017, International Energy Agency (IEA), OECD Publishing, Paris, (2017)
[3] M. Pehnt, H. Helms, U. Lambrecht, D. Dallinger, M. Wietschel, H. Heinrichs, R. Kohrs, J. Link, S. Trommer, T. Pollok, P. Behrens, Elektroautos in einer von erneuerbaren Energien geprägten Energiewirtschaft, Z Energiewirtsch. 35 (2011) 221–234.

[4] F. Cerdas, P. Titscher, N. Bognar, R. Schmuch, M. Winter, A. Kwade, C. Herrmann, Exploring the Effect of Increased Energy Density on the Environmental Impacts of Traction Batteries: A Comparison of Energy Optimized Lithium-Ion and Lithium-Sulfur Batteries for Mobility Applications, Energies 11 (2018) 150.

[5] Z.J. Zhang, P. Ramadass, Lithium-Ion Battery Systems and Technology, in: R.J. Brodd (Ed.), Batteries for Sustainability, Springer New York, New York, NY, (2013) 319–357.

[6] R.J. Brodd, C. Helou, Cost comparison of producing high-performance Li-ion batteries in the U.S. and in China, Journal of Power Sources 231 (2013) 293–300.

[7] VDMA Batterieproduktion (Ed.), Roadmap Batterie-Produktionsmittel 2030: Update 2018, VDMA Verlag GmbH, Frankfurt am Main, (2018)

[8] D. Hall, N. Lutsey, Effects of battery manufacturing on electric vehicle lifecycle greenhouse gas emissions (2018) 1–12.

[9] M. Schönemann, Multiscale Simulation Approach for Battery Production Systems, Springer International Publishing; Imprint: Springer, Cham, (2017)

[10] R. Korthauer (Ed.), Handbuch Lithium-Ionen-Batterien, Springer Berlin Heidelberg, Berlin, Heidelberg, (2013)

[11] T. Kornas, E. Knak, R. Daub, U. Buehrer, C. Lienemann, H. Heimes, A. Kampker, S. Thiede, C. Herrmann, A Multivariate KPI-Based Method for Quality Assurance in Lithium-Ion Battery Production, Procedia CIRP (2019).

[12] S. Thiede, A. Turetskyy, A. Kwade, S. Kara, C. Herrmann, Data Mining in Battery Production Chains towards Multi-Criterial Quality Prediction, Procedia CIRP (accepted for publication) (2019).

[13] M. Westermeier, G. Reinhart, T. Zeilinger, Method for quality parameter identification and classification in battery cell production quality planning of complex production chains for battery cells, in: 2013 3rd International Electric Drives Production Conference (EDPC), Nuremberg, Germany (2013) 1–10.

[14] M. Westermeier, G. Reinhart, M. Steber, Complexity Management for the Start-up in Lithium-ion Cell Production, Procedia CIRP 20 (2014) 13–19.

[15] O. Meyer, C. Weihs, S. Mähr, H.Y. Tran, M. Kirchhof, S. Schnackenberg, J. Neuhaus-Stern, S. Rößler, W. Braunwarth, Development and implementation of statistical methods for quality optimization in the large-format lithium-ion cells production, Energy Technol. (2019)

[16] T. Kornas, M. Z. Karamat, R. Daub, S. Thiede, C. Herrmann, Data- and Expert-Driven Analysis of Cause-Effect Relationships in the Production of Lithium-Ion Batteries, IEEE Transactions on Automation Science and Engineering (accepted for publication) (2019).

[17] A. Kampker, Elektromobilproduktion, Springer Vieweg, Berlin, (2014)

[18] M. Westermeier, Qualitätsorientierte Analyse komplexer Prozessketten am Beispiel der Herstellung von Batteriezellen, Utz, Herbert, München, (2016).

[19] L. Cao, Domain Driven Data Mining, Springer, Dordrecht, (2010).

[20] S. Charaniya, H. Le, H. Rangwala, K. Mills, K. Johnson, G. Karypis, W.-S. Hu, Mining manufacturing data for discovery of high productivity process characteristics, J. Biotechnol. 147 (2010) 186–197.

[21] R. Evans, M. Boreland, A multivariate approach to utilizing mid-sequence process control data, in: 2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC), New Orleans, LA, IEEE, 14.06.2015 - 19.06.2015 1–5.

[22] J. Schnell, C. Nentwich, F. Endres, A. Kollenda, F. Distel, T. Knoche, G. Reinhart, Data mining in lithium-ion battery cell production, Journal of Power Sources 413 (2019) 360–366

[23] L. Schäfer, Analyse und Gestaltung fertigungstechnischer Prozessketten: Konzept zur datenbasierten Ermittlung qualitätswirksamer Einfluss-Ursache-Wirkzusammenhänge und zur Ableitung von Maßnahmen zur Prozesssicherung. Hochschulschrift, Kaiserslautern, (2003)

[24] H. Petersen, Selektion von statistischen Versuchsplänen, ecomed, Landsberg/Lech, (1992)

[25] D. Steuer, Multi-Criteria-Optimisation and Desirability Indices, Universitätsbibliothek Dortmund.

[26] E. Harrington, The Desirability Function, Industrial Quality Control 21 (1965) 494–498.

[27] G. Derringer, R. Suich, Simultaneous Optimization of Several Response Variables, Journal of Quality Technology 12 (1980) 214–219.

[28] C. Shearer, The CRISP-DM Model: The New Blueprint for Data Mining, Journal of Data Warehousing (2000) 13–22.

[29] T.B. Reddy, D. Linden (Eds.), Linden's handbook of batteries, 4th ed., McGraw-Hill, New York, NY, (2011)

[30] G. O. Udu, O. E. Charles-Owaba, Review of Multi-criteria Optimization Methods – Theory and Applications, IOSR Journal of Engineering 10, (2013) 01-14.