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Model-based identification of production tolerances in battery production

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Abstract

Battery technology in combination with carbon-free energy presents a major paradigm shift for the future of the mobility and energy storage sector and already creates an immense demand for large scale battery factories. However, current battery production sites still report considerable scrap rates caused by insufficient process control and a lack of adequate production tolerances, which increase the cost and environmental impact of the battery cells. The present work introduces a methodology which assist in defining model-based production tolerances by considering the impact of varying process parameters on final cell properties in combination with production cost and cell revenue.

Keywords: Modeling; Quality assurance; Tolerance design; Battery production

1. Introduction

Electromobility is increasingly seen as a consistent strategy towards reducing the contribution to climate change from the transport sector. In this regard, the demand for battery cells required is forecasted to increase from 282 GWh in 2020 to 2623 GWh in 2030, which can only be realized with a large number of new battery cell factories [1]. The performance of battery cells must continue to be improved and their production cost must also be reduced to make battery-powered devices marketable solutions. While the latter can be achieved through large scale production and thus exploiting economies of scale, the former can be achieved through innovative cell chemistry, new cell formats and improvements in the production process. The production process in particular still offers great potential for improvement of battery cells, as it is a highly complex system with heterogenous processes and numerous cause-and-effect relations between process and structural parameters along the process chain, many of which are not yet fully understood [2, 3]. In addition to the quantification of the absolute influence of process parameters on the intermediate product and the final battery cell performance, the influence of the deviation of process parameters on the distribution of structural parameters plays an important role. These distributed structural parameters propagate along the process chain and affect the final properties of the battery cells. Consequently, when production tolerances for structural parameters can not be fulfilled, intermediate or final products become scrap. Currently, double-digit scrap rates for battery production are reported which is also a direct consequence of insufficient production precision for quality-critical processes [4]. While it is evident that process capability for quality-critical processes must be further improved, less critical processes might remain unchanged if the production cost for improving precision outweighs the benefit for the final quality of the battery cell. When comparing the effects of production precision on the final quality of the cells, the question arises as to how precisely the individual processes must be set.

In the following, a methodology is presented which enables model-based decision support for production tolerances by

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taking into account both production cost and the effects of production on the final quality of the battery cell.

2. Technical background

2.1. Complexity of battery production

Battery cells are electrochemical energy storage systems. The production process consists of a set of heterogenous process steps which can be divided into electrode production, cell assembly, and cell finishing (Figure 1). The production chain combines processes from different backgrounds, such as process, mechanical, and electrical engineering. While the electrode production is mainly continuous, the cell assembly and cell finishing are mainly discrete. The long process chain exhibits a large amount of process parameters and state variables for the machines (e.g. mixing intensity, foil speed, temperature) as well as various structural parameters and properties of the intermediate and final products (e.g. porosity, coating thickness, energy density). The multitude of heterogeneous influencing factors and the only recent history for large scale applications causes that many effects along the process chain are not fully discovered and understood yet. Kwade et al. provide a comprehensive overview of the current status and challenges for automotive battery production technologies [2].

2.2. Quality improvement in battery production

A high product quality is a decisive aspect during each production process and especially relevant for the automotive battery production due to the high requirements towards their performance and safety. Taguchi loss function suggest it should be measured not by an acceptance rate but by the deviation from a design target value since moving further away from the design target means essentially a loss related to the product [5]. The deviation in final product quality are caused i.e. by the machine, the material, ambient conditions and the operator [6]. Consequently, achieving higher product quality typically requires more accurate machines, more skilled workers or more controlled environments, all of which are associated with higher production costs. Different qualitative and quantitative approaches have been proposed to identify quality-critical parameters in battery production. Westermeier introduced a qualitative approach based on Failure Mode and Effect Analysis which allows to identify cause-effect relations in complex process chains such as battery production. The findings from the qualitative insights can then be used as the basis for further quantitative experiments [7].

In the last years, several data-based approaches were published which help determine the quantitative impact of input parameters on final cell properties. Schnell et al. compares numerous data-mining methods (e.g. generalized linear model, artificial neural networks, support vector regression) for the prediction of final battery cell capacity before the formation process [8]. Turetskyy et al. present a thorough concept on how to acquire relevant data – both automated and manual data – along the production line and then applies the Cross-industry standard process for data mining (CRISP-DM) on the data to rank the importance of different input parameters on final cell properties [3]. Kirchhof et al. [9] and Kornas et al. [10] further extend to the latest development in data-mining in battery production by integrating both data analysis and expert knowledge for ramp-up and production phase to improve fault detection. While the above mentioned contributions focus on the absolute impact of input parameters on final cell properties, other works focus on the highly relevant aspect of deviating process parameters, structural parameters and final battery cell properties. Kornas and colleagues utilize process capability indices for the identification of cause-effect relations and desirability functions allowing for multi-criteria optimization of different quality parameters. Further, Schnell et al. [8] and Turetskyy et al. [11] introduce quality gate concepts in which knowledge of the intermediate product features are used to predict and – if necessary – alter the performance of future battery cells.

Besides data-based approaches, there exist further approaches based on mechanistic models of the production processes and the battery cell. Thomitzek et al. [12] and Schmidt et al. [13] describe a combined mechanistic process chain simulation and pseudo-2-dimensional battery cell model which is used to determine the impact of process parameter deviations on battery cell properties. Other authors developed a Coarse Gained Molecular Dynamics model to describe the structure of the electrode and subsequently use a 3D, respectively a 4D-resolved electrochemical performance model at cell scale. This approach helps quantifying the effect of particle assembly on battery performance with and without including the production process [14, 15].

In conclusion, there exist a wide range of quality management approaches which focus either on the absolute impact of process/structural parameters on structural parameters or battery cell properties. The importance of parameter deviations has been addressed in a few data-based and also mechanistical model-based approaches. While from a product quality point of view, an ever higher production process precision indeed can be a valid goal, the influence of different deviating process parameters on the final battery cell properties can vary immensely. When defining production tolerances, those structural parameters need to be addressed first which have a particular strong influence on the final battery cell quality and/or can be implemented cost-effectively. Altogether, there is a clear demand for a methodology which enables a model-based identification of production tolerances in battery production which considers both the necessary cost and impact of more precise process parameters on final battery cell properites.

3. Methodology

Model-based production tolerances can be identified when the impact of the production precision can be related to the fluctuation of battery cell properties. In addition, the impact of decreasing or increasing production precision must be balanced from both the manufacturing cost and the resulting battery cell revenue (Figure 1).

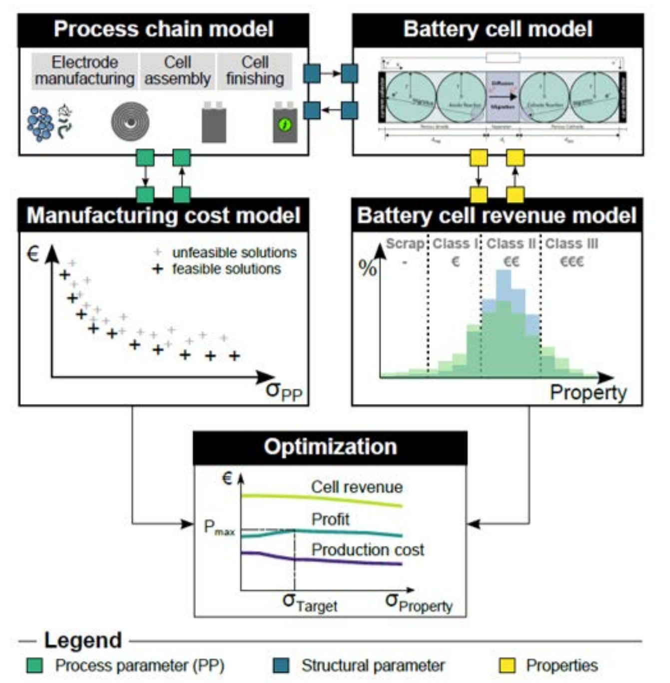

Fig. 1. Methodology for identification of production tolerances based on the application of a manufacturing cost model and battery cell revenue model.

3.1. Process chain and battery cell model

In order to describe the influence of fluctuating process parameters on battery cell properties, a combined process chain and battery cell model is used, which was previously presented in [12] and [13] (Figure 2). The process chain model consists of different mechanistic process models, which reflect the influence of process parameters of the machine on the structural parameter of the intermediate/final product (e.g. line load during calendering on coating thickness of coated substrate). The result of the process chain model is a battery cell characterized by structural parameters which serves as input for the battery cell model. Thereafter, a three dimensional micro structure model based on [16] first determines further effective structural parameters (e.g. effective electric/ionic conductivity). Subsequently, a pseudo-2-dimensional model is used on the basis of these extended structural parameters to calculate performance properties of the battery cell (e.g. energy density, capacity). Since all models consider fluctuating parameters, the effect of process inaccuracies on the structural parameters of the intermediate products and further on the battery cell properties can be regarded. The reference quantity of the combined simulation approach is a single battery cell. Depending on the resolution of the cell, either one or multiple values can be considered to characterize the structure and the properties. Using a simulative approach to describe the process-product interdependencies provides a cost-effective solution to predict the effects of production inaccuracies along the process chain on the final battery cell properties.

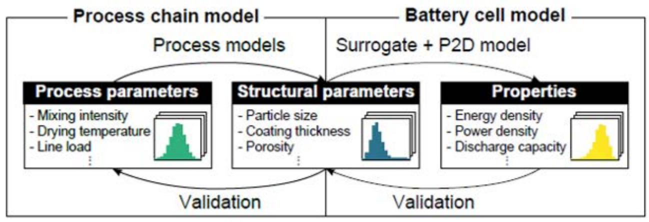

Fig. 2. Combined process chain and battery cell model concept.

3.2. Manufacturing cost model

The manufacturing cost model examines each process of the production chain individually and considers the precision of the machine as a function of the investment and operational machine cost (Figure 3). In general, it is assumed that a more accurate machine, respectively a more accurate operation, results in a higher overall machine costs (investment and operation). The precision of the machine is described by the standard deviation of the respective process parameter $\sigma_{PP,mach}$. Different machines with different accuracies and cost (c_{mach}) can be considered for each process (Figure 3a). The machine precision represents the base value for the process precision. Besides the initial machine precision, also the operation of the machine affects the precision of the process. In the following three different factors (≥1) are examined which may decrease the overall process precision. Each factor is multiplied to the initial standard deviation $\sigma_{PP,mach,i}$, resulting in the final process fluctuation σ_{PP} (Eq. 1).

First, the parameter design affects the precision of the machine. Machines possess ideal design points where their precision is highest (Figure 3b). Beyond these design points, the precision of the machine might decrease. In addition, the sensitivity around the selected process parameter affects the overall machine precision. If possible, process parameters with a low sensitivity (i.e. low gradient) to the precision should be selected, since small deviations from the selected process parameter do not cause greater deviation in precision. The impact of the parameter design is considered by the factor f_{pd}. The parameter design also contributes to the operational cost (c_{pd}) since the process parameter typcially affects the power demand of the machine (e.g. more electrical power required for higher temperature or higher pressure).

Second, the operator can also affect the precision of the process. While an experienced operator is more likely to ensure a precise machine operation, personnel without prior experience (very common in battery production) can cause significant variations in precision, which is accounted for by f_{op_i} (but can improve over time - see Figure 3c). In the manufacturing cost model, the different experience level of the machine operators are reflected by the labor cost c_{op}.

Third, the maintenance of the machine and its impact on the process precision is also considered. In general, machines are maintained in regular intervals to ensure longlasting functionality and precision. Otherwise machine precision would decrease due to wear of machine components and machine supplies. If maintenance intervals are too long or are not performed at all, it is likely that the original precision of the machine will not be achieved after maintenance or the machine precision will keep regressing (Figure 3d). This time-dependent impact of machine wear and the maintenance cost are considered by f_{ma} and c_{ma}.

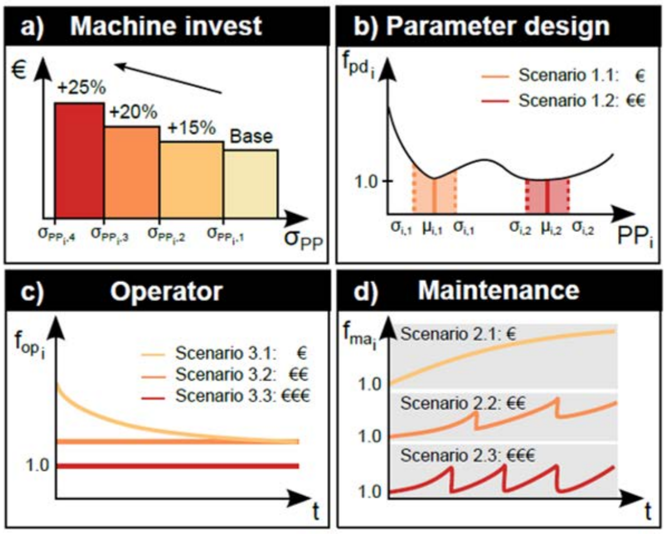

Fig. 3. Manufacturing cost model consisting of four elements: a) selection in machine cost, b) parameter design, c) operator, and d) maintenance.

Each machine typically possesses multiple process parameters i, which is why multiple standard deviations $\sigma_{PP,i}$ can be generated. Consequently, the final precision of the process parameters and the total cost of the machine and its operation can be determined by:

$$\sigma_{PP_i} = \sigma_{PP_{mach_i}} \cdot f_{pd_i} \cdot f_{ma_i} \cdot f_{op_i} \tag{1}$$

$$c_{total} = c_{mach} + c_{pd} + c_{ma} + c_{op} \tag{2}$$

The different scenarios for each element of the manufacturing cost model are combined to consider all possible compositions of the process. Based on Eq. 1 and 2, the respective standard deviation of the process parameter and the total costs are determined. The total cost for the different scenarios are considered for the definition of production tolerances (Sec. 3.4). The standard deviation $\sigma_{PP,i}$ feed as input into the process chain simulation. There, the fluctuating process parameters result in fluctuating structural parameters, which in turn lead to fluctuating battery cell properties. A representative period of simulation time must be considered for the identification of production tolerances since the influence of the operator and the maintenance changes the standard deviation $\sigma_{PP,i}$ over time.

3.3. Battery cell revenue model

Based on the results of the process chain and battery cell simulation (Sec. 3.1), a distribution of differently performing battery cells is generated. Accurate production processes lead to a low fluctuation in the battery cell performance properties and vice versa. These battery cells with fluctuating properties are classified into different quality grades. High-performing battery cells can be used for premium applications and thus be sold at a higher price than low-performing ones. Battery cells that fall below a selected property threshold are considered scrap and do not generate a revenue but could potentially be recycled. Depending on the throughput of the production chain, which depends mainly on production speed of individual machines but could also be extended by increasing the number of production lines and bottlenecks, a total revenue for the battery cells is generated. The revenue is affected by the production precision and thus differs for the respective scenario.

3.4. Identification of production tolerances

Finally, the results from the manufacturing cost and battery cell revenue model are combined to identify production tolerances for each process parameter. While manufacturing cost and revenue both rise with increasing production precision, the revenue increase is typically limited, which results in an optimum for the profit. The scenario with the highest profit provides the suggestions for the machine cost, parameter design, operator, and maintenance selection and essentially predetermines the target production tolerances. When multiple processes parameters are considered (either in a single machine or in multiple machines), this profit-oriented approach helps identifying the process parameter for which a reduction of fluctuation is the most cost-effective. Furthermore, the presented approach takes into account that only those structural variations are reduced which have a direct influence on the fluctuation of battery cell properties.

4. Use case

In the following, the developed methodology is applied to the calendering process of the cathodes. During calendering, the electrodes are compressed to increase energy density and improve physical electrode properties (i.e. porosity, adhesion, conductivity) [2]. Meyer et al. modeled the change in porosity as a function of the process parameters line load q_L and roll temperature T_R [17]:

$$\epsilon_c = \epsilon_{c,0} \cdot \left(p + (1-p) \cdot exp\left(-\frac{q_L}{(\mu_{0\circ C} - \xi \cdot T_R)} \cdot M_c \right) \right) \tag{3}$$

where ϵ_c, $\epsilon_{c,0}$, p, $\mu_{0\circ C}$, ξ, and M_c represent the porosity of the calendered electrode, the initial porosity, a compaction factor, two empirical parameters to determine the compaction resistance, and the mass loading. The coating thickness is described by using a mass balance approach before and after calendering:

$$h_c = h_{dry} \cdot \frac{\rho_{c,dry}}{(1-\epsilon_c) \cdot \rho_s} \tag{4}$$

where h_c, $h_{c,dry}$, $\rho_{c,dry}$, and ρ_s represent the coating thickness after calendering respectively after the previous drying process, the density of the dried electrode, and the density of the coating material. Consequently, the machine precision is determined by the process parameters line load and roll temperature. Both process models are integrated in the process chain model with process and structural parameters from Table 1.

Table 1. Process and structural parameters for calendering process models.

$\epsilon_{c,0}$ [-]	p [-]	q_L $[N\ mm^{-1}]$	$\mu_{0°C}$ $[Nm\ g^{-1}]$	ξ $[Nm\ g^{-1}\ °C^{-1}]$
0.495	0.434	200	1270	2.57
T_R $[°C]$	M_c $[kg\ m^{-2}]$	h_{dry} $[\mu m]$	$\rho_{c,dry}$ $[g\ cm^{-3}]$	ρ_s $[g\ cm^{-3}]$
60	145.5	68.83	2.12	4.19

Three different precision levels are assumed for both process parameters resulting in nine potential calendering machines (Table 2). Higher process parameter precision requires a higher invest.

Table 2. Calendering machine invest as a function of different process parameter accuracies. Reference value for σ_{T_R} and σ_{q_L} = 10% from [23].

	$\sigma_{T_R} = 2\%$	$\sigma_{T_R} = 4\%$	$\sigma_{T_R} = 6\%$
$\sigma_{q_L} = 2\%$	1,932,000 €	1,656,000 €	1,380,000 €
$\sigma_{q_L} = 4\%$	1,848,000 €	1,584,000 €	1,320,000 €
$\sigma_{q_L} = 6\%$	1,680,000 €	1,440,000 €	1,200,000 €

For parameter design, a roll temperature of 60°C and a line load of 200 $N\ mm^{-1}$ are selected with an assumed f_{pd} of 1.02, indicating that the machine precision operates close to its optimum. Power demand and electricity price are 10 kW respectively 0.1 € kWh^{-1}. Three different operator settings are considered with hourly labor cost of 50 €, 40 €, and 25 €. The first two describe experienced operators with a f_{op} of 1.0, respectively 1.1. The third operator assumes an exponential improvement over time with an exponent of 0.01 and a final f_{op} level of 1.1. Finally, a logistic function was selected for the time-dependent maintenance impact f_{ma}, with a maximum value of 3.0, a growth rate of 0.017 and an additional factor for the expontential function of 2. Three different maintenance intervals of 100, 180, and 365 days were selected with maintenance cost of 5%, 3%, and 0% of the relative machine invest.

Overall, nine machines, three operator settings, and three maintenance plans are considered resulting in a total of 81 different scenarios with a simulation time of 365 days. Porosity and coating thickness are passed on to the battery cell model previously described in [13] to determine the properties (e.g. volumetric energy density). Based on a calendering velocity of 30 $m\ min^{-1}$, a production of 4 million battery cells is assumed. Three different quality grades and a scrap are defined for the distribution of the battery cells (Table 3).

Table 3. Classification and market price of battery cells.

Grade	Energy density	Cell price
Class III	> 1850 $Wh\ l^{-1}$	20.0 €
Class II	> 1770 $Wh\ l^{-1}$	18.5 €
Class I	> 1720 $Wh\ l^{-1}$	16.0 €
Scrap	≤ 1720 $Wh\ l^{-1}$	0.0 €

Depending on the fluctuation of the process parameters (input structural parameters in Eq. 3 and 4 are constant), differently performing battery cells are generated for each scenario. Figure 4 shows the different shares of the quality grades depending on the scenario and the volumetric energy density of Scenario 0 and 80. While the proportion of *Class I* and *Scrap* battery cells increase with increasing imprecision, the proportion of particularly high-performance cells also rises. However, when the production processes become less precise (e.g. Scenario 80), the share of battery cells with lower energy densities exceeds the share of battery cells with higher energy densities (distribution is left-skewed). The battery cells with higher energy densities eventually reach the electro-chemical limitations. Therefore, mean energy density decreases with decreasing production precision.

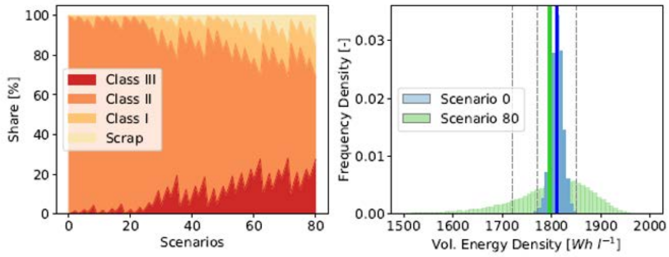

Fig. 4. Share of different quality grades for the 81 scenarios (left) and battery cell volumetric energy densities for the production scenario with the highest (S0) and lowest (S80) precision (right). The vertical lines display the mean volumetric energy density (blue and green) and the threshold for the battery cell grades (grey lines).

Finally, the production tolerances for the calendering process are identified by balancing revenue and calendering cost. The highest profit was determined for the initial process parameter precision of 2% for line load and 6% for roll temperature indicating that the impact of the former is more critical regarding production precision. Further, the most inexperienced operator but the most frequent maintenance plan was selected, reflecting the relative importance. The respective process parameter precisions are determined as production tolerances for the calendering process. Figure 5 illustrates the revenue, profit, and calendering cost for the 81 scenarios. When a standard deviation of 1.5% is exceeded a linear decrease in revenue can be noticed. Standard deviations lower than 1.5% show a nearly constant revenue meaning that an improvement in production precision only provides little benefit. Consequently, the target volumetric energy density and the respective relative standard deviation are 1809 $Wh\ l^{-1}$ and 1.06% resulting in a final calendering cost, revenue, and profit of 1.68, 73.85, and 72.17 million €.

5. Conclusion and outlook

The presented methodology enables to identify the most relevant drivers for variation in production processes providing valuable insight on how to effectively improve the process.

A methodology is presented which enables to identify economically-optimized production tolerances for the battery production chain. For this purpose, manufacturing cost and battery cell revenue are balanced in order to generate the maximum profit. Manufacturing costs consider machine

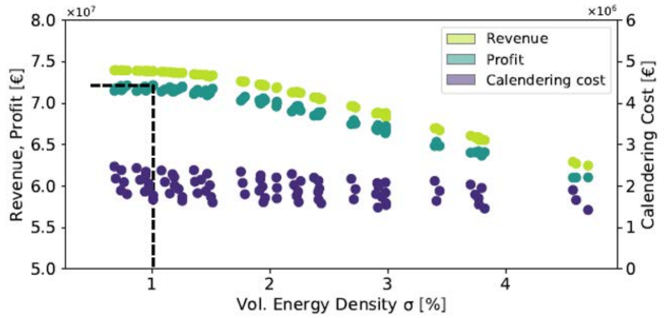

Fig. 5. Revenue, profit, and calendering cost for the 81 scenarios depending on standard deviation of the volumetric energy density.

invest and operational cost (electricity demand, operator, maintenance). Revenue is determined by classifying battery cells according to their properties (e.g. volumetric energy density). The impact of the production process on battery cell properties is quantified using a combined process chain and battery cell model. The production tolerances are derived directly from the fluctuating process parameters that generate the largest profit. The presented methodology allows to identify the main drivers of variation in production processes and provides valuable insights on how to effectively improve the process. By applying the methodology, decision support regarding the machine acquisition and operation can be provided. Accordingly, production tolerances that are too precise can be avoided. The methodology is applied to the calendering process. The results indicate that a decreasing production precision results in lower mean volumetric energy densities since optimum energy density is limited and lower volumetric energy density can continue to decrease downwards. While the methodology is applied on a virtual production, it can also be extended to real production lines.

In the future, the methodology will be extended to multiple processes helping to identify which process precision needs to be addressed first in order to decrease final property fluctuation. Furthermore, the impact of not only fluctuating process but also structural parameters needs to be examined to identify relevant process-product interdependencies along the process chain.

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