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Procedia CIRP 120 (2023) 780–785

www.elsevier.com/locate/procedia

55th CIRP Conference on Manufacturing Systems

Model-based process design under consideration of production performance for battery cell production: A coating and drying study

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Abstract

The production of lithium-ion battery cells is composed of heterogeneous processes, each defined by parameters that influence the properties of intermediate and final products. Due to these complex interdependencies, process variations also affect production performance. Against this background, this works proposes a process design concept that combines process and production-oriented models. The case study investigates different coating speeds and drying temperatures considering process quality criteria, throughput, machine utilisation, and total energy demand. The results show that process-specific changes affect unequally the entire process chain and highlight the importance of a comprehensive approach targeting quality and energy efficiency.

Keywords: modeling; simulation; process design; process chain performance; energy efficiency.

1. Introduction

Lithium-ion batteries are currently the main energy storage technology and their applications include consumer electronics, electric vehicles, and stationary energy storage systems [1]. Therefore, guaranteeing battery cells' quality and economic competitiveness has been the focus of diverse studies over the past years [2–4]. Together with quality improvement and cost savings, the establishment of environmental sustainable production is also a grand challenge of battery cell production [1].

Each process step of battery cell production is characterized by diverse process parameters that affect the intermediate and final product quality [5]. Understanding these process-structure-property interdependencies is essential to achieving higher process and product quality and, consequently, lower scrap rates [6]. Therefore, process design (i.e. the definition or improvement of process parameters) is approached in a variety of works focused on product quality [4, 7, 8]. Since the processes in the battery cell production are strictly interlinked, the parameter interdependencies are propagated and become more complex along the process chain [9, 10]. As a consequence, process-specific changes can affect the entire production, including material flows and energy efficiency [11–13]. Despite its importance, there is a lack of studies that deeply investigate the effects of variations of parameter interdependencies on both product (e.g. intermediate structure) and production (e.g. energy demand, throughput) levels. Considering production performance indicators in process design investigations would contribute to a more comprehensive analysis, including the aspects related to economic and environmentally efficient production.

Against this background, this work proposes a concept of model-based process design in which interdependencies on process and production levels are considered. For that, Section 2 discusses the theoretical background on approaches for investigating process interdependencies in battery cell production. Based on the gaps derived from the state of research, Section 3 presents the concept and its main elements. Lastly, the methodology is applied in a case study for the coating and drying processes in Section 4.

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10.1016/j.procir.2023.09.075

2. Theoretical Background

2.1. Modeling of battery cell production

Battery cell production can be divided into three phases: (i) electrode production, (ii) cell assembly, and (iii) cell conditioning. The cathode and anode process chains are characterized by batch and continuous processes while the last two phases are composed by discrete processes. Besides being strictly interlinked to each other, each process step is characterized by process-structure interdependencies that affect the intermediate and final product quality [2, 6]. As a consequence of this complexity, battery cell production presents scrap rates of approximately 5 % for giga-factories up to 50 % for pilot lines [14]. Furthermore, improvement of yield ratio is essential to the environmental and economic success of battery cell production since the raw materials used in battery cells are associated with high costs and high environmental impacts, due to energy and resource-intensive extraction[6, 14].

Energy efficiency is also critical since processes of electrode production (e.g. coating and drying) as well as cell formation are associated with high energy demands. Moreover, cell assembly is performed under controlled environmental conditions in a dry room that accounts for up to approximately 50 % of the total energy demand [12]. Therefore, strategies to reduce the energy consumption of battery cell production are commonly investigated [9, 13, 15, 16].

Mechanistic modeling and simulation are valuable methods to identify parameter interdependencies since they reproduce of cause-effect relations on process, production, and battery cell levels [8, 17, 18]. Different from data-driven models, mechanistic models are not black-box approaches, do not depend on a large amount of data and can be extrapolated for new scenarios with low experimental costs. Consequently, this method is applied in the planning and design of new processes, production lines, and products [11, 17, 18]. Models on a process level focus on the interactions between process and structural parameters and can be coupled to consider the process chain. For the coupling, parameters related to the intermediate product are exchanged between process models [17, 18]. Production models focus on the material and energy flows between processes along the process chain and investigate the effects of process parameters on the production performance (e.g. throughput, bottlenecks, energy demand) [11, 13, 15]. Lastly, battery cell models investigated the interdependencies between structural parameters and the battery cell performance [3, 9, 17].

2.2. Process design and production performance

Process design (i.e. the definition of process parameters and configurations) aims to improve quality and energy efficiency as well as to reduce costs and environmental impacts associated with production scrap. Due to the manifold of parameter interdependencies in battery cell production, process-structure relations must be understood and quantified to support process design. In this context, modeling and simulation play an important role since they enable a cost-efficient investigation of a large number of parameters [4].

Karaki et al. (2022) present a simulation-based optimization to define process parameters for electrode production under consideration of target structural parameters and production profit. The calculation of production profit also considers production performance indicators (e.g. throughput, energy demand) [3]. Von Boeselager et al. (2022) propose a model-based design solution that combines simulation and experiments in a use case on high-speed feeding and stacking process. The authors further investigate the geometry and position of machine components to support process design. Although high-speed processes aim to increase throughput and productivity, the study does not consider production performance indicators [4].

Further works focus on a production level to investigate the effect of process design on the process chain. Thomitzek et al. (2019) propose a simulation-based approach to assess energy demand in battery cell production. The authors investigate temperature reduction in the calendering process and its effects on energy demand. However, it does not consider the process and product quality [12]. The effects of different drying times on the material and energy flows are also proposed in Schönemann (2017) [10]. In addition, the author investigates the effects of different temperatures. In both scenarios, information on how these alterations affect the process and product quality is not presented.

In summary, studies focused on a process usually do not consider the effects of the process variations on a production level. In addition, studies focused on a production level usually provide a superficial analysis of the effects on a process level, not considering process-structure interdependencies. Therefore, there is a need for a comprehensive process design approach considering a large number of indicators on process and production levels.

3. Methodology

The concept of model-based process design presented in Figure 1 is developed to support the planning and design of new processes or the improvement of existing systems. By implementing this methodology, select scenarios are assessed under consideration of different indicators related to the process quality and production performance.

First, the user defines the boundary conditions of the process of interest. These conditions include target values, technical specifications, and desired parameter ranges which are defined based on production requirements and expert knowledge. Since the main goal of process design is to produce high-quality parts with low scrap rates, target values related to structural parameters (e.g. mass loading) are defined. In addition, technical specifications (e.g. equipment capacity) and feasible processing parameter ranges (e.g. temperature, speed) are defined.

Based on the defined boundary conditions, different scenarios and parameter combinations are specified. These scenarios as well as related structural, process, and production parameters are considered in the second module in which the effects

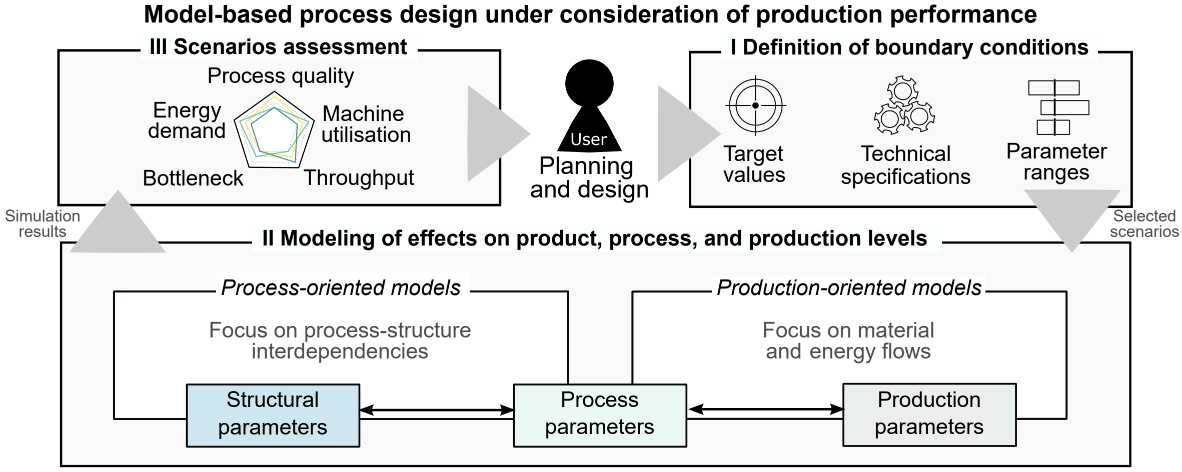

Fig. 1. Concept for process design based on process and production-oriented models.

on process and production levels are modeled. For that, mechanistic *process-oriented models* investigate the process-structure interdependencies. Different models can be coupled via parameter exchange, allowing a process chain approach, as shown in [18]. Diverse modeling methods (e.g. finite element method, computational fluid dynamics) may be developed depending on the process of interest. Based on a combination of discrete event and agent-based simulation [11], the *production-oriented model* investigates interdependencies between process and production parameters. In addition, the effects of process variations on the material and energy flows are studied.

The third module receives the simulation results as inputs for the assessment considering different indicators related to the product, process, and production. *Process quality* comprehends conditions (i.e. coating homogeneity) that are mandatory to achieve the defined target values. The number and type of process quality indicators vary according to the process under investigation. *Machine utilisation* represents the percentage of time in which a machine is processing. Non-processing times include, for example, idle states or failure. *Throughput* comprehends the amount of produced parts on process and production levels. *Bottleneck* investigates the processes limiting the production capacity, leading to long idle times and, consequently, high-energy demand [16]. Lastly, the *energy demand* is investigated on process and process chain levels. The assessment results allow the user to compare the simulated scenarios according to the different indicators. Since a scenario may score differently depending on the considered indicator, criteria prioritization may be necessary. This comparison supports the selection of parameters, process design, and decision-making by the user.

4. Case Study: Coating and Drying

This chapter demonstrates the model-based process design concept in a use case for the coating and drying processes and focuses on two process parameters that influence the material and energy flows along the process chain (coating speed and temperature profile during drying).

For that, mass loading (0.16 kg m^{-2}) and solids content (70 %) are the target values. The main technical specification is a dryer length of 15 m with three zones à 5 m in which the temperature can be adjusted individually. Six stable coating speeds deriving from the coating model are considered as parameter range. In addition, four different temperature profiles (80-80-80, 100-100-100, 80-100-120, and 120-80-100 °C) are investigated. Thus, 24 scenarios are considered in the modeling and assessment. Figure 2 presents the four models considered in the use case.

4.1. Process-oriented models

During electrode production, the slurry is applied onto a current collector in the coating process and subsequently dried. This work investigates the slot-die coating which is a premetered method and provides precise coating thickness at large coating speeds for battery slurries [19, 20]. The coating model is based on the coating window after Schmitt et al. [7] and yields wet-film stability as a quality criterion. This quality criterion is a function of coating parameters (e.g. slot-die geometry, coating gap) and material properties (e.g. viscosity, surface tension) and allows to anticipate successful coating parameters without the need for experiments. The basis of this model is a one-dimensional pressure drop equation of the liquid in the coating underneath the slot-die [7]. The model for investigating the coating stability window obtained from [7] provides the range of feasible coating speeds. Within this range, selected coating speeds are passed to the drying simulation.

The investigated drying process is conducted by a convective dryer [21–23] with three dryer zones with individual temperatures. The model for the simulation originates from the experimentally validated study of Kumberg et al. [24] which has been adapted for the drying of cathodes in prior publications [8]. This model thermally considers the fluid and vapor phase during solvent removal. A combination of heat and mass bal-

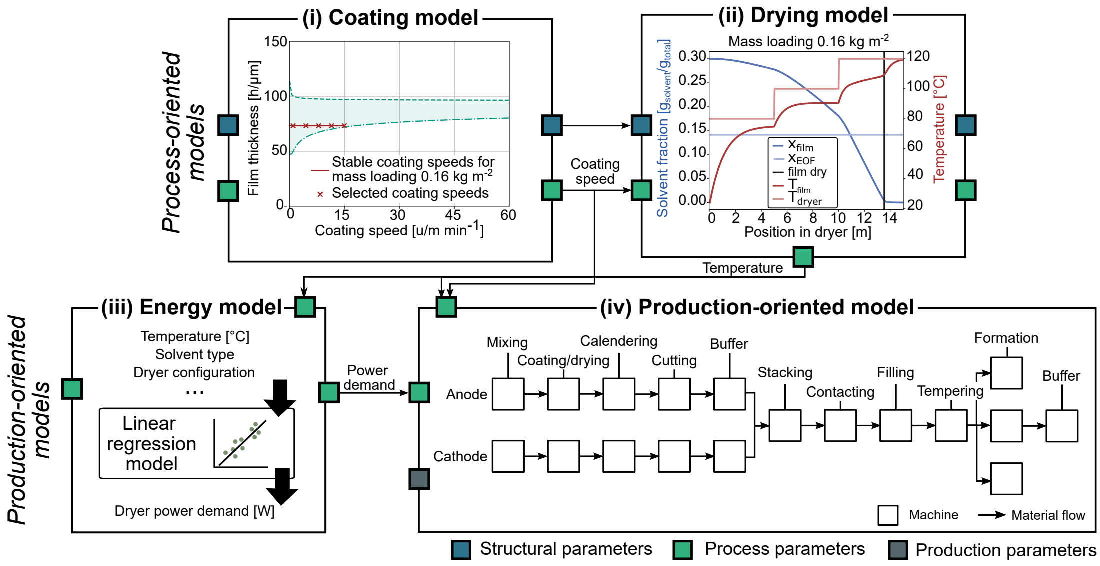

Fig. 2. Process and production-oriented models considered in the case study.

ances, and kinetics results in the solvent loading over time in the dryer. As a result, the usage of dryer space (i.e. the actual dryer length necessary for drying in comparison to the entire length) may be determined. This criterion is assessed by considering the coating speed to predict drying time and position in meter at which the electrode is dry (i.e. drying position).

4.2. Production-oriented models

As explained in Section 4.1, models (i) and (ii) provide two process quality criteria: coating stability and drying position. A higher drying temperature is associated with higher power demand while variations in the coating speed do not have a strong influence on the power demand [25]. Therefore, only the temperature profile influences the power predictions of model (iii). The chosen energy model is a linear regression presented in [3] that considers a 6-meter-long dryer. Since this work considers a dryer length of 15 m, the power demand is linearly scaled up. The production-oriented model (iv) simulates a monthly production of the process chain shown in Figure 2. This model gets feasible coating speeds and temperature profiles from models (i) and (ii) as well as the predicted power demand from model (iii). Only coating speeds and temperature profiles for the cathode production are investigated, i.e. the anode production is not affected. The machines are turned on when input material is available. Further process and production parameters were gathered in the Battery LabFactory Braunschweig, as presented in [2].

4.3. Scenarios assessment

Process quality - Coating stability: The coating stability is the green area plotted in Figure 2 (i). The dashed green lines illustrate the critical film thickness for each coating speed. Thus, coating defects (e.g. swelling, low flow, and air entertainment) may occur if the process parameters result in a production point outside of the green area.

The considered mass loading is equivalent to a wet-film thickness of 73.2 μm. The red line illustrate the stable coating speeds for this wet-film thickness from which six values were selected to be investigated in the dryer and production-oriented models: 1.0, 2.0, 4.5, 8.0, 11.5, and 15.0 m min^{-1}.

Process quality - Drying position: The six stable coating speeds in addition to the four selected temperature profiles resulted in the 24 drying positions shown in Table 1. The intensity of the green color represents how much of the dryer length was used in the process. In addition, the red cells indicate the scenarios in which the quality criterion was not met.

Table 1. Drying position for the different temperature profiles and coating speeds.

Temperature profile	Coating speed [m min^{-1}]					
[°C]	1.0	2.0	4.5	8.0	11.5	15.0
80-80-80	2.4	4.8	9.5	14.9	0.0	0.0
100-100-100	1.2	2.5	5.5	8.8	11.8	14.6
80-100-120	2.4	4.8	7.3	10.3	12.0	13.6
120-80-100	0.8	1.5	3.4	7.6	12.0	14.8

As shown in the table, coating speeds of 1.0 and 2.0 m min^{-1} result in low utilisation of the dryer length since the slurry is dried within the first 5 meters. i.e. the first zone. Three scenarios utilise more than 95 % of the available dryer length and are represented in dark green. Lastly, the electrodes were not dried at the end of the process for the two highest speeds at constant 80 °C. Therefore, these two scenarios were not considered in the energy and production-oriented models.

Two of the temperature profiles that efficiently exploit the dryer length at high coating speeds provide similar results based on the assessment of this study. However, the electrode quality may vary depending of the temperature profile. According to [26], the temperature profile 120-80-100 would result in a structurally better electrode than the ones produced with the temperature profile 80-100-120 °C.

Monthly throughput: This indicator is related to the material flow along with the process chain and is, therefore, not affected by the variation in the coating speed. As shown in Table 2, the increase in the coating speed from 1.0 to 2.0 m min^{-1} results in 50 % more cathodes. This growth stabilizes for the other considered coating speeds. Since the cathode and anode production lines converge into the cell assembly, the throughput of the cathode is limited by the subsequent processes. On the other hand, there is no clear trend for the cell throughput as the values oscillate for the considered scenarios. The formation is a long process and is limited by the machine capacity. Thus, the assembled cells still have to wait a long time to start the formation process although cathodes are being produced faster.

In summary, these throughput values show that changes in one process parameter have effects on electrode production as well as cell assembly. These effects are not similar and are also not proportional to the increase in the coating speed.

Table 2. Monthly throughput of the cathode and battery cell production lines.

Coating speed [m min^{-1}]	1.0	2.0	4.5	8.0	11.5	15.0
Cathode [tsd.]	69	104	104	104	104	104
Cell [-]	624	702	650	676	702	650

Machine utilisation: As the throughput, the machine utilisation is only affected by changes in the material flow. Figure 3 presents the machine utilisation rates for the processes from cathode production, cell assembly and formation. The utilisation rate is calculated based on the total processing time of a machine over the entire simulated period. First, the results demonstrate a large discrepancy of utilisation rates for the different processes. The machines of the cathode production are in a processing state between approximately 40 and 50 % of the a coating speed of 1.0 m min^{-1}. As expected, the values for the coating and drying processes are strongly affect by the different speeds which leads to a sharp reduction of utilisation rates towards increasing coating speeds. As shown in the graph, the values for contacting remain high for all the scenarios which indicate this process being a bottleneck for the cathode production. An analysis of the values for the cell assembly and formation indicates also a non-proportional alteration caused by the increasing coating speeds. Here, the processes tempering and formation also present constant high rates, indicating a limitation of the process chain capacity.

Energy demand: Energy demand is an indicator affected by variations in temperature profiles and coating speeds. Higher

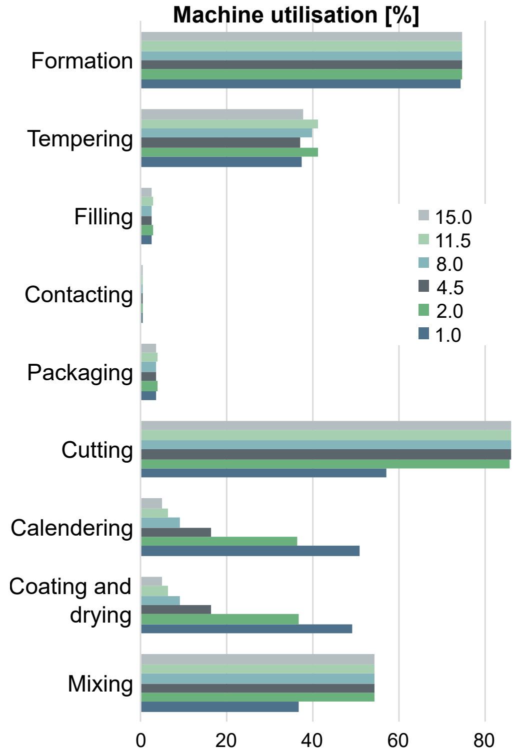

Fig. 3. Machine utilisation rate for a one-month production.

temperatures lead directly to an increase in power demand during drying. As presented in Figure 3, a variation in coating speed cause changes in the machine utilisation and affect, therefore, the processing and waiting times. Waiting times are usually associated with lower power demands, leading to variations in the energy demands on a process and process chain level. Table 3 presents the energy demand per produced cell (i.e. specific energy) for the different scenarios. The power demand for the profiles 80-100-120 °C and 120-80-100 °C are equal to the values for constant 100°C and are, therefore, not included in the table.

A comparison between the different temperature profiles at the same coating speed shows that lower temperatures lead to lower specific energy demand. However, the difference between both profiles is not constant towards variations in the coating speed. Furthermore, increasing the coating speed does not necessarily result in lower energy demand.

Table 3. Specific energy demand [kWh cell^{-1}] for the different scenarios.

Temperature profile [°C]	Coating speed [m min-1]					
	1.0	2.0	4.5	8.0	11.5	15.0
80-80-80	18.1	13.7	11.9	11.1	-	-
100-100-100	19.8	14.6	12.3	19.8	10.9	10.9

5. Conclusion and Outlook

Process design for battery cell production requires a deep understanding of the parameter interdependencies on process, product, and production levels. However, there is a lack of studies considering also the production level and the effects of design choices on production performance (e.g. throughput and energy demand). Against this background, this work proposed a concept for process design that combines models on process and production levels. Based on boundary conditions (e.g. target values, parameter ranges), scenarios are selected and their results are evaluated by considering indicators related to process quality and production performance (e.g. throughput, machine utilisation, and total energy demand). The concept implementation was discussed in a case study for the coating and drying processes. A comparison of the results shows that no scenario scores well in all the selected indicators. Moreover, variations in one process have non-proportional effects on the entire production. Thus, the results highlight the importance of the presented comprehensive approach.

The concept is not limited to battery cell production or to the selected process. Therefore, other studies may focus on expanding the investigated process or the design of other products. In addition, future work will consider the combination of process-oriented models in a process chain approach and further aspects related to material efficiency.

Acknowledgements

The authors gratefully thank the Federal Ministry of Education and Research for funding this work in the project Sim4Pro (grant number 03XP0242B) within the ProZell Cluster.

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