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Simulation-based Assessment of Energy Demand and Costs Associated with Production Scrap in the Battery Production

Simulationsbasierte Bewertung des Energiebedarfs und der Kosten unter Berücksichtigung des Produktionsausschusses in der Batterieproduktion

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Abstract: The shift in the mobility sector towards electric vehicles is responsible for a growth in the market demand for lithium-ion batteries. To follow this trend, the current 200 GWh global production capacity of lithium-ion batteries will present an annual increase up to 300 GWh in the next years. Characterized by an energy-intensive process chain and high material costs, battery production is sensitive to scrap. Current works on energy and cost assessment in the battery production consider scrap rate based on static values derived from historical production data. Thus, there is a lack of works describing the influence of different scrap rates on the process chain dynamics, e.g. machine states and utilisation capacity. To tackle this challenge and contribute to a more cost competitive and environmentally sustainable battery production, this work presents a simulation-based methodology to assess the indirect and direct energy demand and costs associated with production scrap. Based on a combined discrete event and agent-based simulation, scenarios with different scrap rates are simulated. The results show that the effects associated with production scrap varies for each process and are influenced by various factors, e.g. process characteristics, position in the process chain, material costs and energy demand.

1 Introduction

Lithium-ion batteries offer a wide range of applications, with the mobility sector accounting for more than 60% of the 200 GWh global demand in 2019. To follow the electromobility growth, studies predict that the global capacity of production of lithium-ion batteries will present an annual increase up to 300 GWh in the next years (VDMA Battery Production 2020). Due to its energy-intensive process chain, raw material extraction and manufacturing are responsible for up to 45% of the battery cradle-to-gate environmental impacts (Drachenfels et al. 2021). Besides the environmental impact, production is also the main cost driver. Here material is a decisive aspect, accounting for up to 70 % of the costs of a single battery (Kwade et al. 2018). Therefore, a more environmentally sustainable and cost competitive battery cell production depends on a material and energy efficient production. The reduction of production scrap, i.e. material waste intrinsic to the process or resultant from material flaws, increases the material efficiency and reduces the production costs. For large scale production, production scrap rate varies from 5 to 10% (Drachenfels et al. 2021). Different works in the battery production context with focus on energy efficiency (Thomitzek et al. 2019a; Weeber et al. 2020; Erakca et al. 2021) and cost estimation (Nelson et al. 2019; Schünemann 2015; Mauler et al. 2021) consider production scrap in their models and calculations. Nevertheless, the influence of production scrap on the process chain dynamics (e.g. machine states and utilisation capacity) has not yet been discussed. Simulation-based approaches represent a well-established tool for understanding complex relationships and dynamics of process chains, and have already been applied in the analysis of material and energy flows as well as production improvements (Schönemann et al. 2019; Weeber et al. 2020). Against this background, this work proposes a combined discrete event and agent-based simulation approach to (i) dynamically study the effect of different scrap rates on a process chain level and (ii) provide an identification of critical processes from energetic and economic perspectives.

2 Theoretical Background

2.1 Lithium-ion Battery Production

The battery cell production is characterized by a rigidly interlinked process chain with numerous heterogeneous process steps. In general, the process chain can be divided into electrode production, cell production and cell conditioning. However, slight variations might occur in the battery process chain depending on the respective process technology and the battery cell design, e.g. pouch, cylindrical or prismatic. In the electrode production, anodes and cathodes are produced in batch and continuous processes, located in separate production lines to avoid contamination (Schünemann 2015). After a dry and wet mixing process, the respective material suspension is coated and subsequently dried to produce a composite structure. Afterwards, anode and cathode coils are calendered to reduce their porosity, and slit to width and length before they enter the dry room for the cell production, characterized by discrete processes. First, the coils are further cut to single electrode sheets. For pouch cells, the individual electrode sheets are stacked together with a separator. The electrode-separator assembly is contacted internally and afterwards inserted into a pouch bag housing. The housing is then filled with electrolyte and subsequently sealed. In the cell conditioning, the formation and aging of the battery cells are conducted (Kwade et al. 2018). Scrap rate information in the literature is diverse and limited, usually derived from input-output rates and historical data. Based on previous publications, Drachenfels et al. (2021) present variations in scrap rates according to production scales, e.g. 5 - 20 % for small and 5 - 10 % for large factories. Nelson et al. (2019) present process-specific scrap rates, varying from 1 to 8 % according to the process characteristics. Schünemann (2015) proposes even lower rates, e.g. 1 % for mixing process and 0.2 % for stacking. Production scrap rate has also a major influence on production energy demand and costs.

2.1.1 Energetic Perspective

The battery cell production requires a significant amount of electrical energy, especially caused by its energy-intensive processes, e.g. coating/drying, calendering and formation (Thomitzek et al. 2019a). In addition, the technical building services (TBS), which provides the necessary environmental conditions, also contributes to a significant share of the total energy demand (Wessel et al. 2021). The literature reports large variations in energy demand per energy storage capacity at industrial scale, ranging from 47 to 162 Wh per Wh (Erakca et al. 2021). These variations can be explained by the production scale, the complex and dynamic combination of continuous and discrete processes as well as the selected process parameters and boundary conditions (Drachenfels et al. 2021; Thomitzek et al. 2019b). The assessment of energy considering scrap rates has been shown in different works. Thomitzek et al. (2019a) present a material and energy flow analysis based on input-output ratios and the measured energy demand. Weeber et al. (2020) propose a simulation on process chain and process levels to assess the overall energy demand. Wessel et al. (2021) provide an analysis of energy demand due to scrap for a pilot line based on production data. The results show energy-intensive processes as critical when analysing energy demand due to scrap. Although the scrap rate has been considered in many works, it was usually limited to static values based on the average of production data. Thus, it is necessary to analyse closely the influence of scrap rates in battery production on the energy demand, considering process chain dynamics.

2.1.2 Economic Perspective

Material costs represent the largest share of battery production costs. Kwade et al. (2018) present in a cost breakdown that 74.9 % of the costs are caused by material and 3.1 % by energy demand. Duffner et al. (2021) show the share of the various costs for an optimization scenario with materials (77 %), machine depreciation (8 %), production scrap (6 %) and energy (3 %) being the largest ones. Due to the importance of material efficiency for a more competitive production, production scrap has been considered in different cost estimation models. A simulation-based approach to assess the importance of economy of scale on production costs is presented by Mauler et al. (2021) which considers production bottlenecks and end-of-line scrap rate. With regard to process-specific costs, Kwade et al. (2018) declare that processes further down the process chain are more cost sensitive, since they embody the value added by the previous processes. Duffner et al. (2021), on the other hand, mention an electrode production process (coating) as critical. The review on cost models presented by Duffner et al. (2020) lists many works which consider process-specific parameters in their estimations. However, none of them analyses process chain dynamics when defining scrap and energy related costs. Based on the relevance of the material efficiency to the battery cell costs, it is fundamental to consider the economic influence of different scrap rates.

2.2 Simulation Approaches for Process Chain Dynamics

Simulation is a consolidated approach to analyse different production scenarios and process chain performance (Schönemann et al. 2019). In the battery production context, it has also been identified as an effective tool to assess and analyse energy demand for different production and machine configurations (Thomitzek et al. 2019b; Weeber et al. 2020). Discrete event simulation (DE) enables a better understanding and reproduction of material and energy flows within the production as well as provides insights on dependencies between processes. Agent-based simulation (AB) enables to describe elements, e.g. machines or products as unique agent, study their interactions, and store specific data. The use of DE and/or AB to analyse production throughput, machine availability, and process-specific energy demand in the battery context was already proposed by different works (Weeber et al. 2020; Thomitzek et al. 2019b; Schönemann et al. 2019). When considered, scrap rate is described as a process characteristic based on static data to support analysis of input and output flows between processes. Therefore, there is a lack of works with focus on the production scrap rate and its influence on the process chain dynamics.

3 Methodology

A simulation-based methodology was developed to study the influence of different production scrap rates on the process chain dynamics with focus on energetic and economic perspectives, as described in Figure 1.

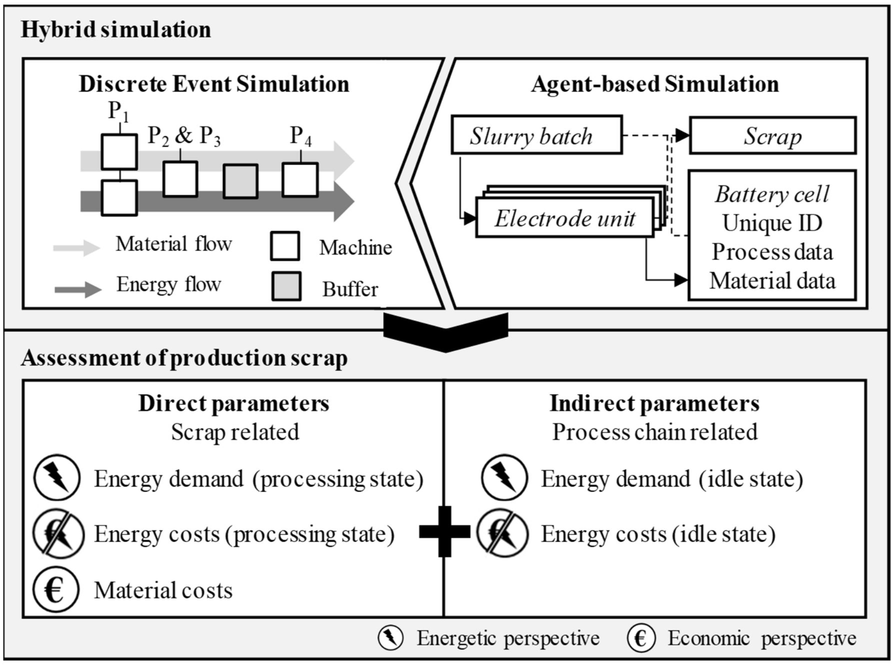

Figure 1: *Simulation-based methodology to assess the effects of production scrap.*

3.1 Hybrid Simulation

The first methodology part is a python-programmed hybrid simulation which combines DE and AB approaches. The focus of the DE is to reproduce material and energy flows of a process chain, consisting of the following elements: machine, process and buffer. A process can be executed by more than one machine and a machine can be associated to more than one process. In addition, it is possible to have buffers to store finished parts. Otherwise, the finished part is temporarily stored in the machine, until it is taken to the next process. A machine presents five states: *off*, *ramp-up*, *idle*, *processing*, and *failure*. *Off* is the machine state either at the beginning of the simulation or after breakdowns. The *ramp-up* state starts after the machine is switched on until it is ready to produce. A machine is in *idle* state before processing, i.e. waiting for input material and machine availability. The *processing* state represents the production itself and, in some cases, the execution of sub-processes and storage of finished parts. Lastly, a machine may fail during processing. Average power consumption and duration are inputs defined by the user and associated to each machine state. An overview on the conditions for state changes and power consumption over time are shown in Figure 2.

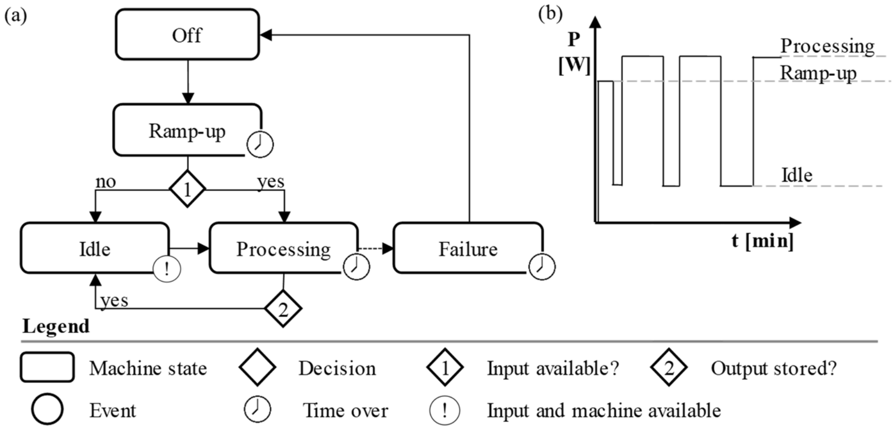

Figure 2: *(a) Machine state chart (b) Machine energy profile based on the duration and average power consumption of the different states.*

The conditions for each state change are represented in Figure 2a. With exception of the off state, all state changes are triggered by an event. *Ramp-up* and *failure* events are time-regulated, based on the user inputs regarding the average and variation of the process duration. The *processing* state is time-regulated and additionally considers the storage of finished materials. The *idle* state is controlled by two events: input and machine availability. The last condition is especially relevant for machines associated to more than one process. The timestamp of changes in the machine states as well as power consumption values result in the energy profile shown in Figure 2b.

The AB simulation focuses on the agents, e.g. slurry batches, electrodes and battery cell. During the simulation, agent-specific information regarding the process (e.g. timestamp and energy demand) and the material (e.g. input, output and scrap ratios) is stored. The interaction between agents is achieved by the possibility to combine them. For example: a battery cell contains various cathodes, these cathodes originate from the same slurry batch. The agents are either located in a buffer or a machine, which provides the integration of both DE and AB approaches. A timestamp is stored whenever a state change in the DE triggers a change in the agent location. Further process and material-specific data, e.g. scrap and output amount as well as energy demand are also stored within each agent. The integration of both simulation approaches provides knowledge regarding the conditions under which each agent is produced and the associated energy demand. The main program functions responsible for this integration are described in Figure 3.

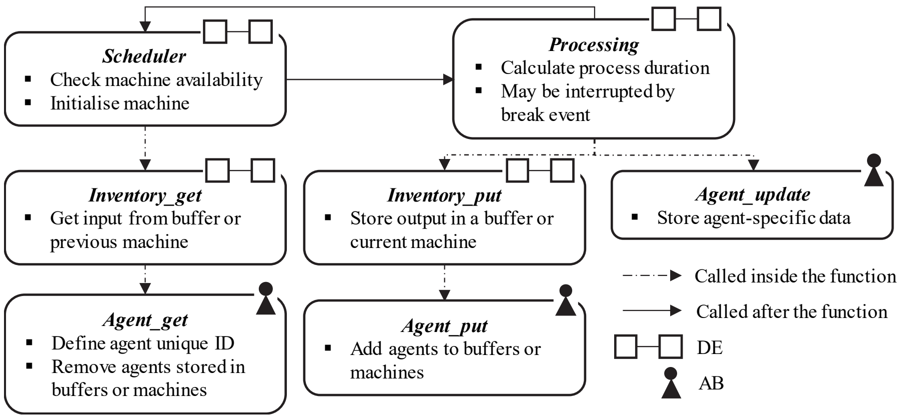

Figure 3: *Program main functions for the DE and AB simulation approaches.*

Scheduler is one of the main functions, responsible for initialising the machines at the simulation start. It is also called before and after processing to check the machine and input availability. The acquisition of input material and storage of finished parts are executed by the *inventory_get* and *inventory_put* functions. These functions are based on the Python package SimPy which enables an allocation of materials in a virtual container and provides, for example, the possibility to wait until a material is available. Lastly, the functions *agent_get*, *agent_put*, and *agent_update* support the AB simulation by managing the creation and location of agents as well as data storage.

3.2 Assessment of Production Scrap

The simulation results are used to assess the energetic and economic influences of different production scrap rates, considering direct and indirect parameters. Different power consumption values are associated to the machine states ramp-up, idle and processing. Energy demand during processing results from the average consumption and duration, and may be directly associated to a scrap agent. As consequence, energy demand during processing state is classified as *direct* parameter. Parameters affected by scrap on a process chain level are classified as *indirect*. Production scrap may cause changes in the material flow and affect the duration of waiting times and energy demand of machines. Therefore, energy demand in idle state is considered an *indirect* parameter. In the battery production, TBS is a major energy consumer, responsible for maintaining adequate production conditions. Since these conditions must always be achieved, independently of the throughput and scrap rate, TBS energy demand is constant and, therefore, not considered in this assessment.

A complete estimation of production costs includes fix and variable costs. Fix costs are associated to investments (e.g. machine acquisition), building, maintenance and overhead. Variable costs comprehend material, energy and labour. Since the fixed costs are strictly dependent on the production scale and are constant regardless of the production throughput and scrap rates, they are not considered in this work. Moreover, for constant working hours and number of shifts, labour costs also remain the same. Thus, material and energy are the only costs considered in this assessment. Material and processing energy costs are classified as *direct* since they are calculated based on agent-specific information, e.g. amount of scrap and energy demand. *Indirect* parameters comprehend the ones affected by scrap on a process chain level, i.e. energy costs related to idle states.

4 Use Case: Battery Cell Production

The proposed methodology was applied to the pilot line of the Battery LabFactory Braunschweig (BLB). The energy and process parameters for the pouch cell production were automatically acquired via the SCADA system described by Turetskyy et al. (2020). Since material prices for a pilot line are not consistent to the ones for a larger production scale, this use case considered the prices described in the BatPac cost model (Nelson et al. 2019). An around-the-clock production with the BLB machine capacities was simulated to investigate the dependencies and dynamics between processes, e.g. share of each machine state as well as material and energy flows. Moreover, differently from the BLB pilot line, the simulation considered separate production lines for cathode and anode production, as shown in Figure 4.

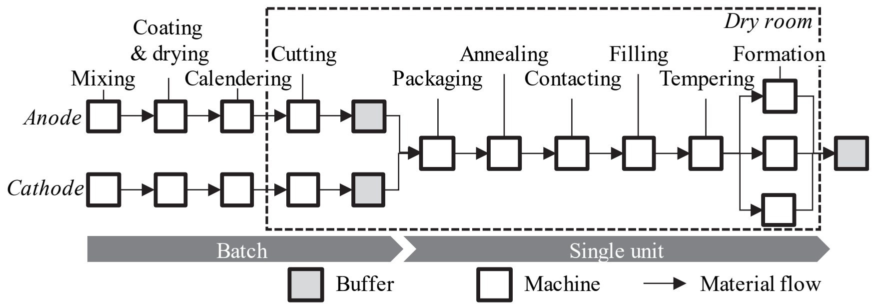

Figure 4: *Simulated processes adapted from the BLB production line.*

First, a one-month production with no scrap was simulated as a base scenario. Subsequently, the simulation was repeated in four scenarios with scrap rates ranging from small to large scale productions (1 %, 5 %, 10 %, and 15 %). In each scenario, the same scrap rate was considered for every process which represents, for example, a yield of 90.4 % for the 1 % scenario. For batch processes, scrap is a share of the produced batch. For single unit processes, scrap represents a complete unit.

4.1 Results and Discussion

The simulation results of all the five scenarios were assessed according to the direct and indirect parameters described in the methodology. First, the influence of scrap rate on a process chain level was evaluated by measuring the variation of indirect parameters for each scenario. The energy cost for the entire process chain associated with production scrap was calculated based on the energy demand in idle state per finished (good and scrap) part [kWh per part] of each process and the electricity price for business in Germany of 0.237 $ per kWh. To provide a better identification of the variations, the costs for idle and processing states are compared in Figure 5.

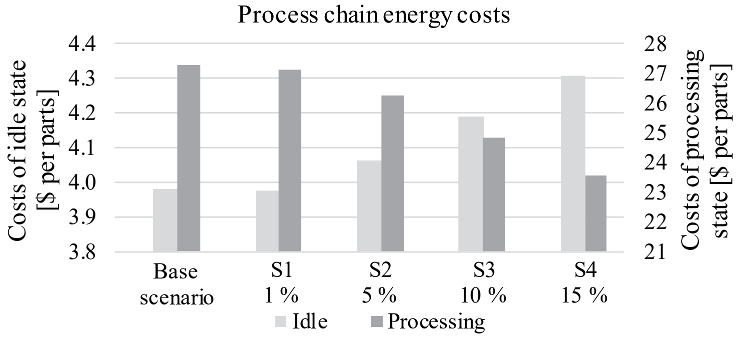

***Figure 5:** Costs associated with energy demand in idle and processing states for a one-month production for the base scenario and different scrap rates.*

These results reinforce that a variation in the scrap rate is responsible for a change in the process chain dynamics. Since the processes are rigidly interlinked and the throughput of each single unit process is reduced by an increase in the scrap rate, processes down the process chain have to wait longer for input material. This increase in waiting times leads to higher idle state costs. The reduction of throughput at each single unit process also leads to fewer processed parts in one month and, consequently, to a reduction in processing state costs. It is also important to emphasize that these effects are not proportional to the scrap rate: for the 15 % scenario, the costs of idle state increase 8.2 % while the costs of processing state decrease 13.6 % in comparison to the base scenario. After assessing the indirect parameters, i.e. influence of scrap rate on a process chain level, the direct parameters were analysed. For this purpose, the energy demand associated with processing and material costs for each scrap agent at each process were calculated. Table 1 presents the total average of material and energy costs per finished (good and scrap) parts for each simulation scenario.

***Table 1:** Direct material and energy costs associated with the different scrap rates.*

	S1 - 1%	S2 - 5%	S3 - 10%	S4 - 15%
Material [$ per part]	11.05	79.90	205.36	289.16
Energy [$ per part]	0.19	1.39	3.05	4.43
Formation finished parts	390	338	260	208

As expected, a scrap rate increase is directly related to higher material and energy costs associated with the production of these parts. Although a uniform increase is seen on the total costs per part, a deeper analysis shows variations in the critical processes for the different scenarios, as represented in Table 2. While some processes are more critical from an energetic perspective, others are more sensitive to material costs. For a 5% scrap rate, cathode calendering and formation are the most critical processes from an energetic perspective. Cathode mixing and formation, on the other hand, are more critical with regard to material costs. Considering the combination of both aspects, the most critical ones are formation and cathode calendering. For the highest simulated scrap rate (15%), cathode calendering and mixing are the most critical processes from an energetic perspective; cathode mixing and filling from a material one. In total, cathode mixing and calendering are the most critical ones.

Table 2: *Comparison of the most critical processes considering direct parameters for 5 and 15 % scrap rates.*

	Mixing Cathode (5%)	Calendering Cathode (5%)	Formation (5%)	Mixing Cathode (15%)	Calendering Cathode (15%)	Formation (15%)
Energy [$]	0.07	0.17	0.19	0.50	1.24	0.31
Material [$]	12.25	1.44	12.21	108.31	11.00	20.57
Total [$]	12.32	1.61	12.40	108.81	12.24	20.89

Variations on a process level change in different proportions for different scrap rates. For batch processes, the number of produced batches remains the same, however, the percentage of scrap is higher. Therefore, electrode production processes are more sensitive to higher scrap rates. Moreover, cathode and anode production present different variations, since cathode production is more intense from both energy and material cost aspects. Overall, the results show that different scrap rates have dynamic effects on the process chain, altering the material flow and the shares in processing and idle times. An analysis on process level shows that processes are affected differently from both an energetic and economic perspective. The intensity of these effects is influenced by the process characteristics (e.g. batch or single unit), position in the process chain, material costs and energy demand.

5 Summary and Outlook

Material efficiency is fundamental for a more cost competitive and environmentally sustainable battery production. Current works on energy and cost estimations consider production scrap rates as static values derived from historical data and do not assess their effect on the process chain dynamics. To tackle this challenge, this work proposed a simulation-based methodology to dynamically study the effect of different scrap rates on a process chain level and provide the identification of critical processes from an energetic and economic perspective. First, a discrete event and agent-based simulation studied the material and energy flows of a one-month battery production. The results for different scenarios were analysed with focus on indirect parameters on a process chain level (e.g. energy demand and costs for idle states) affected by production scrap. In addition, parameters with a direct relation to production scrap (e.g. material costs and processing energy) were assessed. The assessment showed that the effects are different for each process and influenced by various factors, e.g. process characteristics, position in the process chain, material costs and energy demand. Future works will study the effect of process-specific scrap rates to define acceptable tolerances and support the planning of quality gates.

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