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

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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 of up to 300 GWh in the next years. Characterized by an energy-intensive process chain and high material costs, battery production is sensitive to production scrap rate. Current works on energy and cost assessment in battery production consider scrap rates based on static values derived from historical production data. Thus, there is a lack of works that dynamically analyse the influence of different scrap rates on the process chain, e.g. considering machine states and utilisation capacity. To tackle this challenge and contribute to more sustainable and competitive battery production, this work presents a simulation-based methodology to assess the indirect and direct energy demand and costs associated with production scrap.

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 of up to 300 GWh in the next years [1].

Due to its energy-intensive process chain, manufacturing is responsible for up to 45% of the battery cradle-to-gate environmental impacts [2]. 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 [3]. Therefore, a more environmentally sustainable and cost-competitive battery cell production depends on 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. However, reducing the scrap close to zero requires sophisticated strategies and significant investments [4].

For large-scale production, production scrap rates vary from 5 to 10% [2]. Different works in the battery production context with a focus on energy efficiency [5–7] and cost estimation [8–10] consider production scrap in their models and calculations. Nevertheless, there is a lack of works that dynamically analyse the influence of different scrap rates on the process chain, e.g. considering machine states and utilisation capacity. 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 [6,11].

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 identification of critical processes from energetic and economic perspectives.

1 Theoretical Background

1.1 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 electrode production, anodes and cathodes are produced in batch and continuous processes, located in separate production lines to avoid contamination [9].

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 cell production, characterized by discrete processes. First, the coils are further cut into 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 cell conditioning, the formation and aging of the battery cells are conducted [3].

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 to 20% for small and 5 to 10% for large factories [2]. Nelson et al. (2019) present process-specific scrap rates, varying from 1 to 8% according to the process characteristics [8]. Schünemann (2015) proposes even lower rates, e.g. 1% for the mixing process and 0.2% for stacking [9]. Production scrap rate has also a major influence on production energy demand and costs.

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 [5]. In addition, the technical building services (TBS), which provide the necessary environmental conditions, also contribute to a significant share of the total energy demand [12].

The literature reports large variations in energy demand per energy storage capacity at an industrial scale, ranging from 47 to 162 Wh per Wh [7]. 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 [2,13].

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 [5]. Weeber et al. (2020) propose a simulation on process chain and process levels to assess the overall energy demand [6]. Wessel et al. (2021) provide an analysis of energy demand due to scrap for a pilot line based on production data [12]. The results show critical energy-intensive processes when analysing energy demand associated with scrap. Although the scrap rate has been considered in many works, it was usually limited to static average values based on production data. Thus, it is necessary to dynamically analyse the influence of scrap rates in battery production on the energy demand.

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 [3]. 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 [14]. Due to the importance of material efficiency for 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 rates [10]. Concerning 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 [3].

Duffner et al. (2021), on the other hand, mention an electrode production process (coating) as critical [14]. The review on cost models presented by Duffner et al. (2020) lists many works which consider process-specific parameters in their estimations [15].

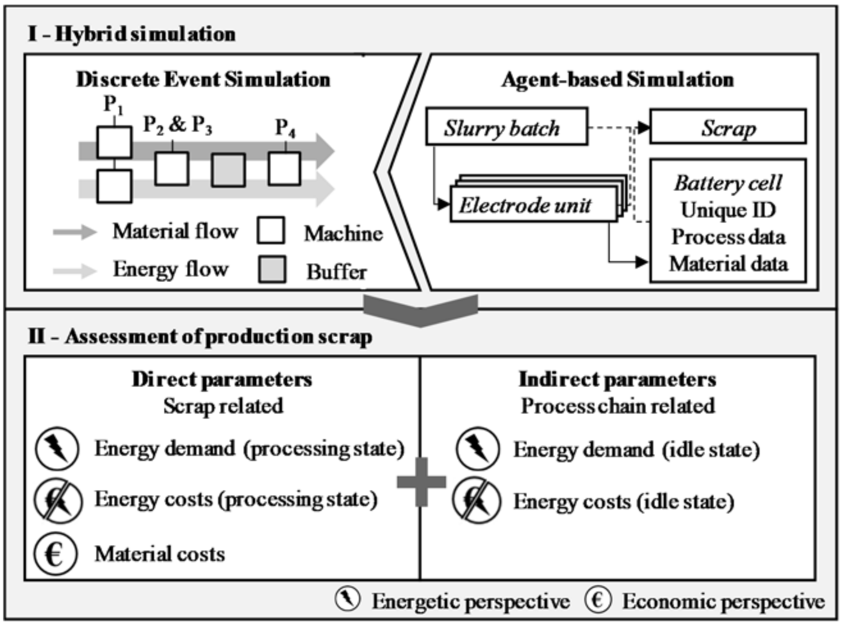

Figure 1: Simulation-based methodology to assess the effects of production scrap on the process chain.

However, none of them dynamically analyses the process chain 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.

1.2 Simulation Approaches for Process Chain Analysis

Simulation is a consolidated approach to analyse different production scenarios and process chain performance [11]. 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 [6,13]. 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 a 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 [6,11,13]. 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 work with focus on the production scrap rate and its influence on the process chain.

2 Methodology

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

2.1 Hybrid Simulation

The first methodology part is a python-programmed hybrid simulation that combines DE and AB approaches. The focus of the DE is to reproduce the material and energy flows along the 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 assigned 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 storage of finished parts. Lastly, a machine may break during processing. Average power consumption and duration of each machine state are inputs defined by the user. An overview of the conditions for state changes and power consumption over time are shown in Figure 2.

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.

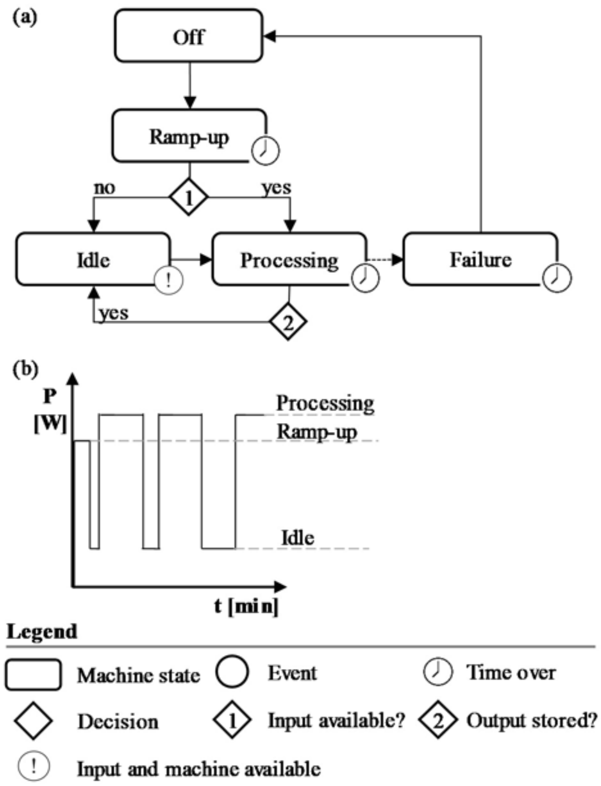

Figure 2: (a) Machine state chart and (b) machine energy profile based on the duration and average power consumption of the different states.

The last condition is especially relevant for machines associated with 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 change. 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.

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 the 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.

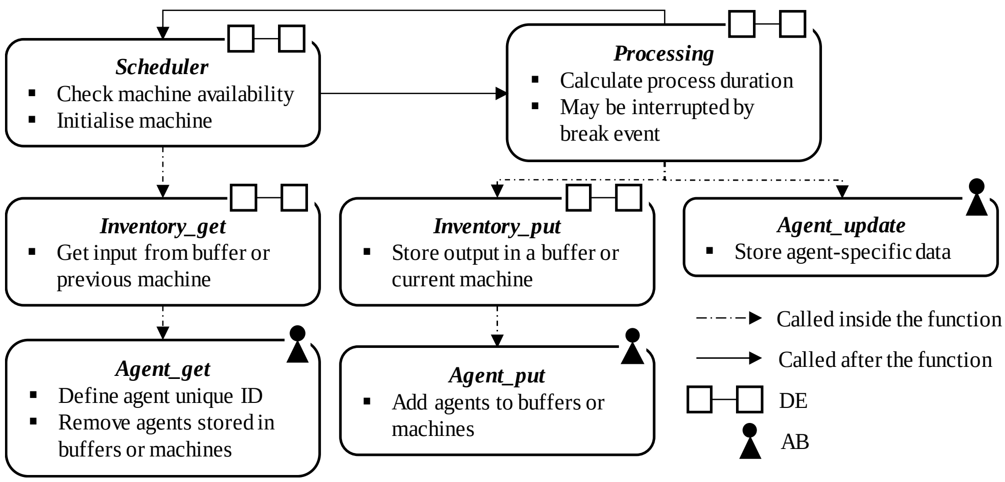

Figure 3: Program main functions for the DE and AB simulation approaches.

2.2 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 with the machine states ramp-up, idle, and processing. Energy demand during processing results from the average consumption and process duration, and may, therefore, be directly associated with a scrap agent. As consequence, energy demand during the processing state is classified as direct parameter. Parameters affected by scrap on a process chain level are classified as indirect. Production scrap may cause, for example, 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 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 with 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.

3 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 to produce a 10-compartments pouch cell were automatically acquired via the SCADA system described by Turetskyy et al. (2020) [16].

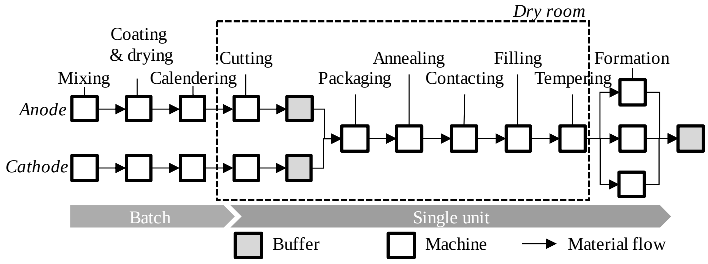

Figure 4: Simulated processes adapted from the BLB production line.

Since material prices for a pilot line are not consistent with the ones for a larger production scale, this use case considered the prices described in the BatPac cost model [8]. 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.

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 an entire unit.

The simulation results of all five scenarios were assessed according to the direct and indirect parameters described in the methodology. First, the influence of different scrap rates was evaluated by assessing the *direct parameters*, i.e. the scrap-related energy demand as well as energy and material costs.

Figure 5 presents the average material and energy costs associated with scrap per finished battery cell for each simulated scenario.

As expected, a scrap rate increase is directly related to higher material and energy costs associated with scrap to produce one battery cell. However, this increase is not proportional to the scrap rate and affects differently the energy and material costs. For the 1% and 5% scenarios, the energy costs are slightly higher than the material costs. For the 10% and 15% scenarios, material costs become more significant.

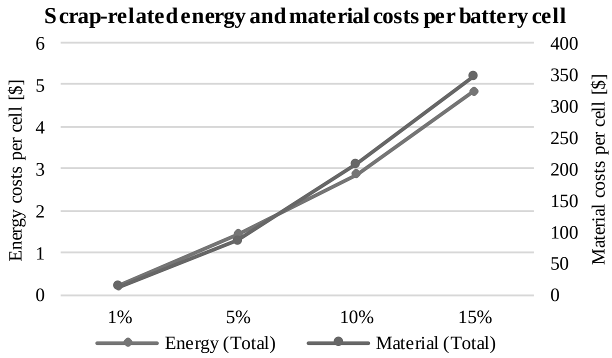

Figure 5: Scrap-related energy and material costs to produce one 10-compartments battery cell for the different simulated scenarios.

		Scrap-related costs per cell [$]		
		Energy	Material	Total
5% scrap rate	C. Mixing	0.001	0.192	0.193
	C. Calendering	0.003	0.022	0.025
	Formation	0.194	12.206	12.400
15% scrap rate	C. Mixing	0.011	2.380	2.391
	C. Calendering	0.027	0.242	0.269
	Formation	0.585	38.567	39.152

Table 1: Comparison of the scrap-related costs for selected processes considering direct parameters (energy and material costs) for 5 and 15% scrap rates.

A closer look at the process-specific costs shows that some processes are more critical from an energetic perspective, while others present significant material costs. The production type (batch or single unit) also plays an important role in the intensity of the scrap effect at each process.

Moreover, cathode and anode production present different variations, since cathode production is more intense from both energetic and material perspectives. Table 1 exemplifies the process-specific variations for one produced battery cell based on three selected processes (cathode mixing, cathode calendering, and formation).

Considering the selected processes of the cathode production, calendering is the most critical one from an energetic perspective while mixing is the most critical one with regard to material costs for both the 5 and 15% scenarios.

Since cathodes are produced in batches, the energy and material costs related to one battery cell (containing 10 cathodes and 10 anodes) are significantly lower than the costs incurred in the single unit processes of cell production, e.g. formation. Regarding the total costs, the most critical processes for both scrap rates are cathode mixing and formation. Furthermore, a comparison of the variations between the 5% and 15% scenarios shows that the total cost of mixing increases by a factor of twelve while the formation total costs by a factor of three.

In a second step, 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 was calculated based on the energy demand [kWh] in idle state for a finished battery cell and the electricity price for business in Germany of 0.237 $ per kWh. To provide better identification of the variations for each scenario, the share of costs for idle and processing states are compared in Figure 6.

The results of Figure 6 reinforce that a variation in the scrap rate is responsible for dynamic changes in the process chain, e.g. duration of machine states. 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 times and costs. It is also important to emphasize that these effects are not proportional to the scrap rate: in comparison to the base scenario, the share of costs in the idle state increases by 1.8% and 10.2% for the 1% and 15% scenarios, respectively.

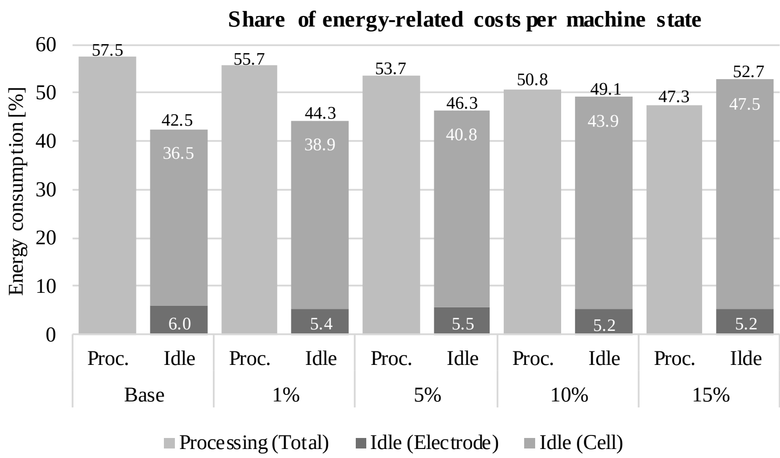

Figure 6: Costs associated with energy demand in idle and processing states per finished battery cell for different scrap rates.

The share in idle states also differs between the electrode and cell production. As shown in Figure 6, the share in idle state for electrode production decreases at higher scrap rates. Since scrap in the electrode production leads to a reduction of the batch size, processes whose duration depends on the material quantity (e.g. coating and calendering) present shorter processing times and, consequently, lower idle times. As previously mentioned, single unit processes need to wait longer for input from the previous processes, therefore, presenting a higher share in idle state at higher scrap rates.

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 the 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 type (e.g. batch or single unit), position in the process chain, material costs, and energy demand.

4 Summary and Outlook

Material efficiency is fundamental for 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 dynamic effect on the process chain.

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 was used to study the material and energy flows of one-month battery production. The results for different scenarios were analysed with a focus on parameters with direct relation to production scrap (e.g. material costs and processing energy).

In addition, the effects of production scrap on a process chain level were assessed based on indirect parameters (e.g. energy demand and costs for idle states). The results demonstrated the importance of dynamically assessing the effects of scrap rates since they differ for each process and are 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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