

Chapter 2

Battery Production and Simulation

This chapter introduces relevant background information about the production of battery components and the assembly of battery systems (Sect. 2.1) as well as about how simulation can be used to imitate the behavior of production systems (Sect. 2.2).

2.1 Battery Production

A sound understanding of the production of batteries requires background information about the structure and components of batteries (Sect. 2.1.1), general knowledge about production systems and production management (Sect. 2.1.2), as well as a description of specific characteristics and requirements of the production of batteries and their components (Sect. 2.1.3).

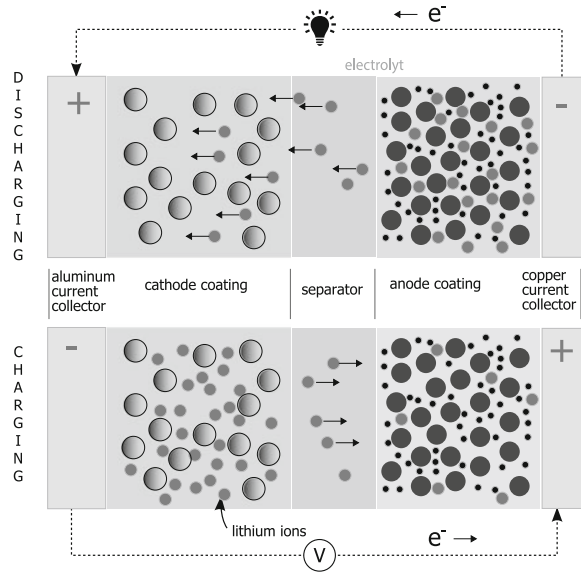
2.1.1 Batteries and Battery Components

As stated in the introduction, until today, the most relevant battery type for large applications is the LIB. LIB systems are commonly used for EV, stationary storage units and consumer electronics. Although new battery types and materials combinations are in development in order to improve the performance of batteries, LIB are expected to stay highly relevant (Kampker 2014). For this reason, the remainder of this section will focus on LIB.

Principle of Lithium-ion Battery Cells

LIB are chemical energy storage systems which transform the stored energy into electricity at electrodes. A basic LIB cell consists of a negative (anode) and a positive (cathode) electrode which are separated by an isolating separator and surrounded by an electrolyte. During discharging, lithium ions move from the anode through the separator to the cathode and bind to active material particles. Simultaneously,

Fig. 2.1 Illustration of the layers of a battery cell



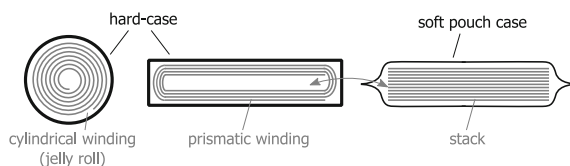
released electrons are conducted through an external circuit from the anode to the cathode. During charging, the direction of the movement of electrons and lithium ions is reversed by a connected power supply. Figure 2.1 illustrates these reactions and the structure of a LIB cell.

Electrodes consist of metallic current collector foils which are coated with active material. The collectors of anodes are usually made of copper while cathode collectors are made of aluminum. Different active materials can be used for anodes and cathodes. These materials are characterized regarding energy density, life time, safety, costs and environmental impacts. It is important to identify material combinations which result in the desired technical properties and cause relatively low costs and environmental impacts. Moreover, different materials require different processes or process parameters, which may also effect costs and environmental impacts.

According to Kaiser et al. (2014), it is important that active materials and pores of active materials are completely wetted and filled with electrolyte so that ions can be released, transported and bound to all active material particles. This avoids local current peaks. Furthermore, it is necessary to contact and bind the active material particles with each other and the current collector to ensure electron transport from and to each particle. The coating layer thickness and active material loading must be uniform to avoid cell failures due to inhomogeneities. Similar rules are stated by Pettinger (2013).

Cells can be designed to provide high energy or high power (Kampker 2014). High energy cells are characterized by high specific energy and low specific power and they usually have thick electrodes with a high density. High power cells are characterized by high specific power and low specific energy and have thin and porous electrodes. While the power of a cell is influenced by the contact area of electrodes, the energy

Fig. 2.2 Cross-sections of types of electrode-separator package and cell housing



content depends on the amount of active materials within one cell (Väyrynen and Salminen 2012).

In addition, cell types can be differentiated regarding their form and housing. The most common types are cylindrical or prismatic hard-case or prismatic pouch cells (Wöhrle 2013; Fleischer et al. 2012). Cylindrical cells usually have a metallic hard-case and an electrode-separator assembly in form of a cylindrical winding (also called jelly roll). Prismatic cells also have a hard-case but with a prismatic flat-winding or a prismatic electrode-separator stack. Pouch cells – also called coffee bag cells – consist of prismatic stacks or windings surrounded by laminated aluminum foil which fixates the bundle of electrodes and separators. Figure 2.2 illustrates cross-sections of the types of electrode-separator package and cell housing.

Kampker (2014) and Pettinger (2013) present the advantages and challenges of the different cell types. Pouch cells can have high specific energy and good cooling characteristics, low weight, and allow a high packing density. Challenges in the development and production of pouch cells exist regarding leak tightness, stacking of electrode sheets, internal pressure, mechanical stability, and production costs. Cylindrical cells can have high specific energy, are relatively easy to produce by winding processes and provide good mechanical integrity, have a high degree of tightness and a high life expectancy. However, their form bears the risk of high temperatures (which requires external cooling), results in a low achievable packing density, and requires additional mounting devices in cell modules. Prismatic cells have a leak tight housing with high mechanical stability and enable an efficient space utilization and easy assembly in cell modules.

In summary, battery cells consist of different components and their characteristics are influenced by the selection of materials (for active materials, collector foil, separator, electrolyte), design parameter (e.g. coating thickness), geometry and housing (e.g. prismatic or cylindrical, soft or hard case), and required production processes (e.g. winding or stacking and related cutting processes). The design of a battery cell has to account for the specific intended use-case and technological, economic and environmental objectives.

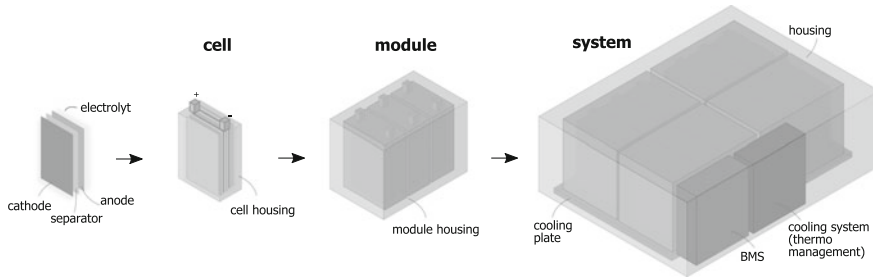


Fig. 2.3 Illustration of an exemplary battery system structure

Structure and Components of Battery Systems

Batteries usually consist of multiple battery cells which are – depending on the intended purpose – connected in serial or parallel which results in higher capacity or voltage compared to single cells (Köhler 2013). Larger battery systems commonly have a modular structure in which several battery cells are combined within modules and several modules are installed in a mechanical structure together with sensors (for monitoring the charge, voltage, and temperature), a battery management system (BMS), a communication interface, a cooling system, and power electronics (Väyrynen and Salminen 2012; Kampker et al. 2013; Warner 2014). Figure 2.3 illustrates a schematic of the structure and components of an exemplary battery system.

Battery modules should consist of cells having matching capacities according to defined tolerated capacity limits. This is important since the capacity of a module is limited by the cell with the lowest capacity (Kenney et al. 2012; Kampker 2014). This is caused by the BMS which will stop charging of a module as soon as the first cell is completely charged. Consequently, all other cells will not receive a full charge (Warner 2014). Moreover, modules should be designed around stackable frames which create a rigid structure and enable a variable length of modules (Väyrynen and Salminen 2012). Furthermore, the design of modules has to consider the used cell type (Fleischer et al. 2012). Pouch cells are flexible to some extent and not as rigid as hard case cells. For this reason, they have to be fixated within the module structure. Additionally, internal pressures may result in bloating of cells so enough space has to be provided in order to avoid mechanical stress. Prismatic cells can be arranged in a more compact manner since the cells are more rigid, require no special fixation and do not tend to expand much during operation. Cylindrical cells are directly fitted to a module chasing. Due to their round form, it is important to position the cells very closely to not waste available space. This is possible since cylindrical cells are rigid and do not expand.

In summary, cells are assembled into modules which must be designed according to the cell type and the desired capacity, current, and voltage. Battery systems consist of various modules and components and can be of different size and shape depending on the intended use-case and the used cell type.

2.1.2 Production Systems and Production Management

The production of battery cells and the assembly of battery modules or systems take place in production systems. The detailed analysis of the production of batteries and battery components requires a general understanding of the typology and management of production systems.

Processes and Process Chains

The actual production is characterized by a physical transformation process which combines input factors into outputs. Inputs to processes are resources and equipment, materials, energy, labor and information which are transformed into desired (e.g. electrodes) and undesired (e.g. waste, emissions) products (Schenk et al. 2014; Dyckhoff and Spengler 2010). Figure 2.4 drafts a production processes with related inputs and outputs.

Complex products – such as batteries – are usually produced by several processes. Such sequences of processes are often referred to as process chains which consist of multiple processes connected through material flows. Process chains can be of different structure referring to the type of material flow which can be classified as continuous, converging, diverging, or rearranging (Dyckhoff and Spengler 2010). Figure 2.5 presents the different types of process chain structures based on the material flow.

In addition, the production activity can further be differentiated regarding type and principle. The production type is determined by the product quantities. In this regard, it is differentiated between the single production of individual products, the repeated series production of a small quantity of a product type or of batches of a defined larger quantity of a product type, as well as the (open end) mass production of a large quantity of product units (Westkämper and Zahn 2009; Dyckhoff and Spengler 2010; Schuh 2006). In contrast to unit processes, which result in one or multiple discrete

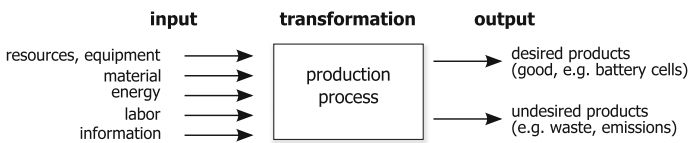


Fig. 2.4 Production as physical transformation process according to Dyckhoff and Spengler (2010) and Schenk et al. (2014)

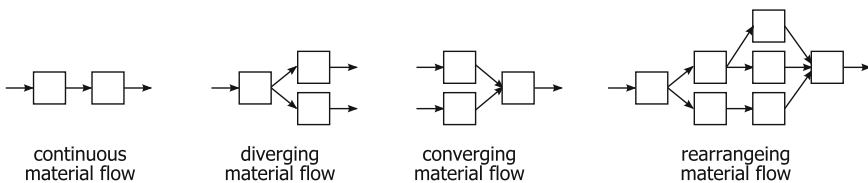


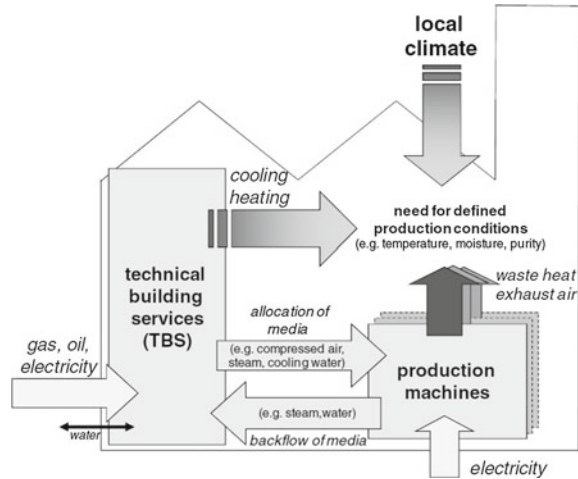
Fig. 2.5 Types of material flows according to Dyckhoff and Spengler (2010)

product units, processes can also be continuous, resulting in batches or a specific amount of product per time period (e.g. Schuh 2006). The production principle can be differentiated regarding the spatial alignment of the processes. In a workshop production, machines for similar operations or processes are grouped together in one area. Products or work pieces have to move to the required workshops. In order to reduce the material flow, machines can also be grouped as cells in one area based on the process requirements of specific product types. Alternatively, machines can be arranged linearly according to their position in a required process sequence. The material flow can be realized for example by transfer lines which create a continuous flow based on a defined tact time or an asynchronous flow. Flexible production systems combine the advantages of the cell arrangement with an automated processing and material flow. These principles and types of production are usually applied in suitable combinations. For example, while workshop or cell configurations are suitable for the production of individual products or small batches of various product types, continuous line configurations are suitable for mass production. Flexible production systems are used for mass production or series production of several product types.

Elements and Hierarchy of Production Systems

Processes and process chains require peripheral processes and equipment, energy and media supply, infrastructure for transport and quality control, worker for operations of machines and material handling, as well as a surrounding workshop space in a factory (Westkämper 2006). Thus, in a greater context, process chains are embedded in production systems. A system in general consists of different entities interacting with each other to fulfill the systems purpose (Westkämper and Zahn 2009). This is also the case for production systems, where system entities (e.g. machines) interact to create products. The elements of factories can be grouped into production equipment, technical building services (TBS), and the building whereas the production equipment can be further linked to single processes or process chains (Thiede 2012). Figure 2.6 shows the structure of these elements which is proposed by Thiede (2012). These elements are connected through flows of material, media, energy, and information which – similar to the actual processes – have to be controlled in order to react on induced changes in the production system (Westkämper and Zahn 2009). For this reason, Westkämper and Zahn suggest a hierarchical structure of production systems which enables defined interfaces between different system elements and a hierarchical target system. Literature provides various concepts for defining the hierarchy of production systems (Wiendahl et al. 2007; Liang and Yao 2008; Verl et al. 2011; Benkamoun et al. 2014; Heinemann et al. 2012; Schenk et al. 2014; Herrmann et al. 2010; Nyhuis and Wiendahl 2010). For example, Wiendahl et al. structure the hierarchy into plant, production area, production system, manufacturing cell, and workstation. According to Westkämper and Zahn (2009), production networks include different factories with production segments, where specific process chains consist of machines or aggregated production cells. Heinemann et al. (2012) differentiate between four levels: factory, material flow (process chain), single process and machines. Similar hierarchies are presented in Herrmann et al. (2010) and

Fig. 2.6 Holistic factory definition from Thiede (2012)

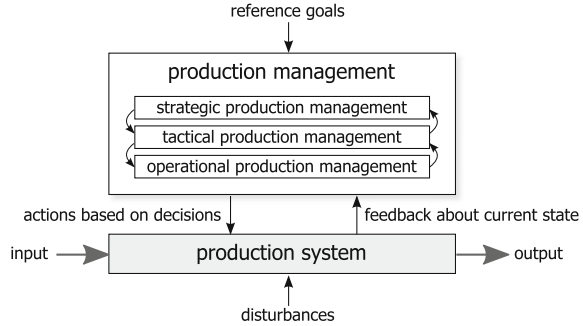


Verl et al. (2011) additionally including the supply chain or global production system as the highest level above the factory level. Schenk et al. (2014) present a hierarchy of sub-systems of a production system based on peripheral orders. Another kind of hierarchy is developed by Nylund and Andersson (2010) by introducing the terms macro, meso, and micro level to production systems. The macro level refers to the behavior of the whole factory including all production stages, material and information flows, layout design and the systems overall performance. The meso level refers to individual production stages consisting of areas with multiple units and their interactions. The micro level refers to units such as machines, tools, methods and work pieces. The authors describe the interactions between the levels as services such as requests and delivery of relevant information. Their concept appears to be the only one directly considering product units with their specific features. Other hierarchy concepts do not specifically include the product level. However, the consideration of products is important in order to describe and investigate product specific routing or material flow as well as the effects of processes on product characteristics. Wuest et al. (2013) developed a more detailed structure of the product level and the interaction between product characteristics with processes. In summary, the examined publications suggest very similar structures for the hierarchy of production systems – although in some cases using different terms – which can also be used to structure the elements of battery production.

Production Management

Industrial production systems must be continuously adapted to short and long term changes in production technology, market, politics and legislation, and society (Dyckhoff and Spengler 2010). The purpose of production management is the design, planning and control, as well as monitoring of the production activity (Schuh and Schmidt 2014). The planning aims at the design of the production system and each individual system element while the control regulates the execution of production activities according to the order management. The production management acts as

Fig. 2.7 Control loop of production management; figure adapted from Dyckhoff and Spengler (2010), Nyhuis and Wiendahl (2010), and Thiede (2012)



the controller in a control loop containing the production system as the controlled system. The control variables are decisions regarding required actions and measures. These decisions can consider strategic, tactic, and operational perspectives. The strategic production management aims at adapting the production system to the requirements of the surrounding environment based on normative and strategic reference goals (e.g. cost or sales objectives). Examples of strategic decisions are initialization of new product development activities and the selection of new facility locations. The tactical production management is responsible for the realization of the strategic decisions. Examples are the utilization of new production technologies or the rearrangement of a factory layout. The purpose of the operational production management is to ensure the production of the requested quantity of products in the desired quality in the available time. Decisions regarding all perspectives have to consider feedback from the production system which is acquired based on defined performance indicators. Examples of feedback variables from the production system are the utilization, production costs, throughput times, and order fulfillment. Figure 2.7 illustrates an abstract control loop with the production system and production management.

More detailed descriptions about production management can be found for example in Schuh and Schmidt (2014), Herrmann (2010), Nyhuis and Wiendahl (2010) and Westkämper (2006).

2.1.3 Production of Battery Cells and Systems

The information about production systems and production management can be used to further investigate the production of LIB electrodes, cells, modules, and systems.

Production of Electrodes and Cells

The production of a LIB cell can be structured into the three stages electrode production, cell assembly, and electrical formation. The major value is added within the cell production stage. However, this stage also requires the highest investment (Roland Berger Strategy Consultants 2010).

The production of battery cells requires many processes in a sequential order. The configuration of process chains for battery cells depends on the cell type, electrode materials, used processes and production technology, as well as on producers specific decisions. There are strong interrelation between different processes and process parameters (Kaiser et al. 2014; Kampker 2014; Gallagher and Nelson 2014; Pettinger 2013; Brodd and Helou 2013). For example, raw materials may be prepared within an intensive dry mixing processes prior to wet mixing (dispersion). As another example, the coating may be continuously or intermittently which also effects the separation process. The separation process further depends on the form of the electrode-separator assembly. Windings require a continuous electrode foil while prismatic stacks need separated electrode sheets. These examples show, that process chains for cells can be rather different and that it is not possible to define a generic reference process chain. However, Fig. 2.8 presents an attempt of a generalized process sequence for cell production based on information from various publications. First, the anode and cathode are produced by mixing, coating of the resulting slurry onto the current collector foil and successive drying, calendaring of the coated foil, separation to required width or the final electrode format, and drying of the finished electrodes. Second, electrodes are used as the basis for the assembly of cells.

Material preparation and mixing The different materials for electrodes such as active materials, carbon black, binder (usually polyvinylidene fluoride (PVDF)) and solvents (e.g. N-methylpyrrolidone (NMP)) are weighted, combined, and mixed in different processing steps. In the mixing processes, first active materials and additives such as carbon black are mixed (Wieser et al. 2015). Next, the prepared materials are mixed with further additives such as a binder and a solvent. The solvent is used to adjust the viscosity of the slurry (Tran et al. 2012; Li et al. 2011a). The desired result of the mixing processes is a viscous slurry which will be coated onto the current collector foil. The material composition of the slurry is different for anodes and cathodes as well as for different cell chemistry systems. Different formulations for the compositions of material types are possible for anodes and cathodes of which an overview (of cathode formulations) is presented by Li et al. (2011a). Different mixing intensities, types of mixing tools, and temperatures can be used to adjust the slurry according to the desired properties such as homogeneity or viscosity (Kampker et al. 2013). The properties of a slurry

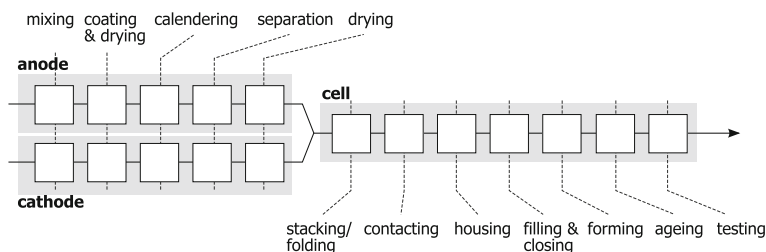


Fig. 2.8 Process chain of lithium-ion battery cells for stacking or folding cell assembly

do not only directly influence the characteristics of the final cell but also the further processing of the slurry in the subsequent process steps (Kaiser et al. 2014).

Coating and drying The slurry is coated onto a current collector foil either on one or both sides. This process significantly affects the product quality. A uniform transmission of the slurry and a defined mass load are required along the length and width of the coating layer (WZL und VMDA 2012b). Different coating methods can be used for applying the slurry onto the foil such as slot-die, comma or roll coating whereas the slot-die coating is the most used method (Schmitt et al. 2013; Kampker et al. 2013). The coating layer can be either continuous or intermittent and it is possible to coat both sides of a foil simultaneously or subsequently. The coating layer must be created with high precision regarding layer thickness and the weight per area unit.

Directly after coating, the layer must be immobilized and solidified via evaporation of the solvent in the following drying process. Different types of dryers can be used and the temperature profile within a dryer has influence on the adhesion of the coating layer to the foils and on the binder distribution across the layer cross-section. Undesired effects caused by wrong process parameters are the detachment of active material particles from the foil which may result in reduced battery performance and higher risk of failures. From an economic perspective it is of interest to reduce the required drying time and increase the throughput, since the process has a high energy demand and long dryers require high investment. Further details about coating and drying can be found in Kaiser et al. (2014).

Calendering The resulting coating layers are usually porous. For this reason, calendering can be used to compact the layer, reduce the pore volumes, and increase the density. In a calender, several rolls are used to gradually reduce the thickness of an electrode (WZL und VMDA 2012b; Kampker et al. 2013). This improves the contact between particles and the foil. Relevant process and machine parameters are compression rate, line force, roller speed, and roll diameters (Haselrieder et al. 2013). Tolerances in coating and calendering can only be accepted on micrometer scale. Larger deviations may result in accelerated aging of the battery cells. This is also the case if anodes or cathodes from upper and lower tolerance limits are combined within a cell (Kaiser et al. 2014).

Separation and drying Depending on the kind of cell packaging, the compressed electrodes have to be separated. The created electrode coils are usually cut to width in a continuous slitting process using rotary knives or lasers (Pettinger 2013; Luetke et al. 2011). The cutting lines must be straight, clean, and precise. The accepted tolerances are small since electrode sheets within one cell must be of equal size. If cells are created by stacking or z-folding, single electrode sheets have to be cut out of the electrode stripes or coils by die cutting or laser cutting (WZL und VMDA 2012b; Baumeister and Fleischer 2014). The separated electrode sheets or coils are dried to eliminate any water content from the coating layer. The following cell assembly is located within a dry room to avoid new water input after drying (Kaiser et al. 2014).

The assembly of battery cells depends on the type of cells to be produced. Especially packaging and housing are influenced by the form of the electrode-separator assembly and the housing.

Package assembly The cell assembly starts with the packaging in which anodes, cathodes, and separator are combined to wrapped packages. The design of the packing process depends on the cell type. Electrode stacks can be created by a stacking or z-folding process. In a stacking process, separate anode, cathode and separator sheets are placed above each other in the order separator, anode, separator, cathode. The stack is completed by sheets of separator, anode, and separator. In a z-folding process, single electrode sheets are placed alternating with a continuously supplied separator (Schmitt et al. 2014; WZL und VMDA 2012b). Cylindrical and prismatic windings are created by a winding process. As in stacking, the order of layers is cathode, separator, anode, separator. Relevant process parameters are tension, positioning accuracy, and angular velocity of the strips and the radius of the windings. The resulting electrode-separator package is wrapped and fixated (Kampker et al. 2013; Baumeister and Fleischer 2014).

Contacting, housing, and filling with electrolyte The tabs of the electrodes of a created package must be contacted. Usually, ultra sonic spot welding or laser welding is used to create the connections (Kampker et al. 2013). Next, the package is placed within the cell housing which is closed and sealed. The cell is filled with a liquid electrolyte. The electrolyte must penetrate into the porous separator and electrode layers. This process is time consuming since the air inside the cell structure can escape only slowly. For this reason, the cells are usually filled and finally sealed under vacuum conditions (Schmitt et al. 2015).

Forming and aging The forming process – the first charging of a cell – activates the active materials and initiates the forming of a solid electrolyte interphase (SEI) on the anode (Yoshio et al. 2009). After the first charge, further charging and discharging cycles can be used to age the cells and to identify cells with reduced performance. Processes parameters are amperage, temperature differences, and pause lengths. The forming and aging processes are among the most energy intensive processes in cell production. Moreover, forming and especially the subsequent aging step are very time consuming. At the end of forming and aging, cells are checked and tested regarding their performance and self-discharge (Hettesheimer et al. 2013).

Assembly of Modules and Systems

The assembly of modules and systems strongly depends on the specific product variant. For example, the cell type, the number of cells per module or modules per system, as well as the design of the housings determine the required production steps. However, an exemplary assembly structure can be characterized based on the descriptions of WZL und VMDA (2012a,b), Kampker et al. (2013), and Fleischer et al. (2012), as shown in Fig. 2.9.

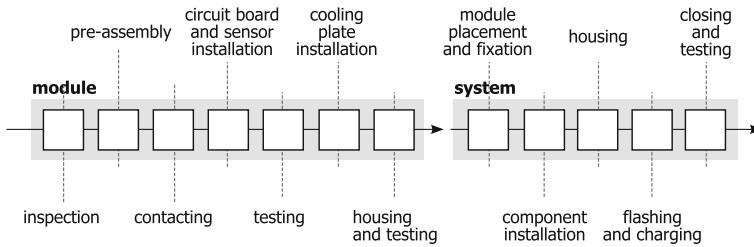


Fig. 2.9 Process chain of battery module and system assembly

At first, the cells are inspected and cells with similar characteristics are clustered. Cells with undesired characteristics are sorted out. Next, several selected cells are pre-assembled on a base plate using fixtures or frames (Väyrynen and Salminen 2012). The cell tabs are contacted according to the desired type of interconnection (serial or parallel). Afterwards, a cell supervision circuit board is installed along with sensors for temperature and state of charge (SOC). The sensors must be wired and connected to the circuit boards. The installed sensors and the circuit board are checked for correct functioning by connecting the module to a power source. In addition, a thermal imaging camera can be used to monitor the welds (WZL und VMDA 2012a). After testing, cooling plates are mounted to the assembly which is inserted into a housing. The final assembly is tested regarding functioning and performance (voltage test) and leak tightness of the cooling system (pressure test). After a visual inspection, a module is completed.

Several modules are used to assemble a battery system. In the first production step of system assembly, selected modules are inserted and mounted into a battery pack base plate. Furthermore, installed are a cooling system, a BMS, and a high-voltage module, as well as the required cables and wires. Next, the BMS is flashed with software for battery management and diagnosis. The latter software is used within a test to analyze the battery operation. Also, an initial charging creates an uniform SOC for all cells. Afterwards, the housing is closed, sealed, and tested regarding leak tightness.

Ambient Conditions for Battery Production

Battery factories must fulfill the high requirements regarding safety and product quality while aiming at low production costs. The production of cells has specific requirements regarding ambient indoor conditions and cleanliness in building zones since temperature, humidity, and cleanliness have significant impact on product quality, safety, performance, and life time of the battery cells (Simon 2013). Simon provides detailed information about the required environmental conditions for the different productions steps in cell production and system assembly. As an example, the cell assembly (and especially the filling with electrolyte) requires low humidity with a dew point temperature up to $-60\text{ }^{\circ}\text{C}$ corresponding to a relative humidity below 1% in the temperature range of $22 \pm 2\text{ }^{\circ}\text{C}$. Consequently, the building construction and building services (e.g. cooling towers, ventilation units, dehumidifiers, heating and cooling) play an important role in the planning and operation of factories

and they contribute to a great share of investment and energy demands. Furthermore, battery factories need the supply of media which are directly required by processes such as water for the production of coating materials, process exhaust air, cooling water and compressed air (Simon 2013). Another relevant aspect mentioned by Simon is the high waste heat from the drying process of the coated electrodes which could be re-used by heat-recovery processes.

Production Costs of Batteries

As mentioned in the introduction, the production costs of a battery system can contribute to up to 40% of an EV which makes them a significant cost driver. The total costs of a battery consist of the costs of raw materials, the process steps in production of electrodes and the assembly of cells, modules, and systems, as well as of other components such as sensors or electronics (Fleischer et al. 2012). During the last few years, several cost models have been developed for modern battery cells and systems (Schünemann 2015; Nelson et al. 2012, 2015; Petri 2015; Petri et al. 2015; Patry et al. 2015; Gallagher and Nelson 2014).

The Battery Performance and Cost Model (BatPaC) was developed at the Argonne National Laboratory (Gallagher and Nelson 2014; Nelson et al. 2012). It supports the design of battery systems. The production steps are separately documented which allows modifications in the cost calculations. Furthermore, the model considers a base plant scenario which can be scaled to represent different output. The impact of flexibility in plants was further studied in Nelson et al. (2015). However, the BatPaC model neglects energy costs and differences between production technologies. Based on the cell design module of the BatPaC, Patry et al. (2015) developed a cost model for cells which breaks costs down into purchase costs, processing costs, overhead costs and other fees. The processing costs are determined based on factors and battery characteristics such as electrode thickness. However, the process cost factors are not explained in detail. Schünemann (2015) provided a more detailed discussion of different existing cost models and developed an own integrated cost model for the production of LIB cells. This model is based on a process chain analysis considering detailed process characteristics and using average values for energy consumption, processing times and material fractions per cell. However, dynamic interactions are not considered within the process chain or the factory level and the model assumes a constant output of cells for the allocation of indirect costs. His results show that a large cost share is already caused in the mixing process due to high material costs. This underlines the importance of eliminating scrap in the following processes.

In summary, the presented models show that battery costs are mostly influenced by the used materials. Differences and uncertainties exist regarding the actual processing costs (e.g. energy costs) and the effect of a higher factory output.

Environmental Impacts of Battery Production

Several LCA studies directly or indirectly have analyzed the environmental impacts of battery production (Ellingsen et al. 2014; Dunn et al. 2014; Hawkins et al. 2013; Notter et al. 2010). Most of these studies evaluated batteries in the context of EV. The study of Hawkins et al. (2013) has shown that the production of vehicle batteries

contributed to 35–41% of the GWP of the entire vehicle production. Their results show a rather high impact of the battery compared to other studies (e.g. compared to Notter et al. 2010), which are found to be caused by different assumptions regarding the energy demands in battery production and different system boundaries. Dunn et al. state that the throughput of a factory has a strong influence on the energy intensity of battery production. This is explained by the high energy demands of energy intensive TBS equipment (e.g. dry rooms) of which the energy demand is independent of the produced quantity of batteries. If the output increases and the energy demand per product unit decreases, the raw material production has the largest influence on the environmental impacts (Dunn et al. 2014). Both of these factors can be influenced within product development and production. Ellingsen et al. recommended reducing the production energy demand or utilizing cleaner energy sources, enabling material recycling, and enhancing the life time of batteries (Ellingsen et al. 2014).

In conclusion, although these studies came to differing results regarding the exact environmental impact, all show that battery production has important influences on the environmental impact of EV. Uncertainties exist mostly regarding the energy requirements of battery production, the throughput of battery factories, and the life time of batteries.

2.2 Simulation of Production Systems

This section describes the role of simulation in the context of the digital factory (Sect. 2.2.1), gives background information about different simulation approaches (Sect. 2.2.2), and about how they are applied in the context of production systems (Sect. 2.2.3). The section explains that the simulation of an entire production system demands a multiscale simulation approach (Sect. 2.2.4) and how co-simulation can support the collaborative development of comprehensive simulation models (Sect. 2.2.5).

2.2.1 *Digital Factory*

The term digital factory¹ refers to a network of digital methods and tools supporting the planning, realization, and improvement of factories including the related processes and products (Westkämper et al. 2013; Bullinger et al. 2009; VDI 2008). Moreover, the term refers to the totality of employees, software, and workflows required to realize the virtual and real world production. Consequently, digital factory is more than just a collection of methods and tools. It is also a set of organizational measures aiming at creating a better understanding of the operation of factories. The main purpose of the digital factory is the predictive, visual and simulative imitation

¹In German: Digitale Fabrik.

of the production of future products. With this function, it acts as a link between product development and production management (Bracht et al. 2011). Moreover, the digital factory aims at improving communication and collaboration between the stakeholders in planning by providing a redundancy-free, consistent data and knowledge base (Landherr et al. 2013). This leads to the goal to establish standardized tools and models which can be re-used within different planning steps such as the planning of factory buildings and TBS equipment, shop floor layout, production processes, logistics and material flow, logistic oriented product development, and machine configuration (Bracht et al. 2011). There are different types of methods to support these different planning tasks. However, according to (Bracht et al. 2011), there is no established structure for methods and tools in the context of digital factory. He defines the following classes of methods: Methods for collecting data and information, methods for design and representation, mathematical methods for analysis and optimization, simulation methods, artificial intelligence methods, methods for visualization as well as for collaboration. In contrast to static methods for analysis and representation, simulation is a method for analyzing complex dynamic effects and interactions. It enables the replication of the time-dependent behavior of factories.

2.2.2 *Simulation*

Simulation is an established method for supporting planning tasks in industry and research. The main principle of simulation is the emulation of an existing or planned system and its behavior over time by using an approach (Banks et al. 2010). This enables gaining insights about the modeled systems behavior which is transferable to the real system (VDI 2014). A system can be defined to be a set of interacting entities. Interactions determine the effect of system inputs on the outputs as well as on states of the system. The entities and interactions have to be included in a formal model which can be executed during a simulation run. Experiments consisting of simulation runs usually support planning tasks or decisions in which different scenarios of system variants have to be evaluated and compared (März et al. 2011).

In general, modeling types can be grouped according to different characteristics (Banks et al. 2010). While discrete models describe the change of system state variables only at events at discrete points in time, continuous models describe system variables continuously over the simulation period. Models can also combine both characteristics and contain discrete and continuous objects within a hybrid model. Furthermore, models can be based on deterministic inputs and deliver repeatable results or contain random variables and determine their values during simulation runs based on random number generators. Moreover, models can be static or dynamic whereas static models describe the state of a system at a specific point in time, often considering stochastic effects (e.g. Monte Carlo experiments, in which models with random variables are repeatedly executed). Dynamic models describe the behavior of a system over time.

In addition to these characteristics, four main simulation approaches can be differentiated which are suitable for different levels of abstraction of the related models (Borshchev and Filippov 2004).

Discrete event (DE) simulation uses passive entities which flow through a network of resources and trigger actions and variable changes. In DE models, states of the modeled system change at discrete points in time. This approach is usually used on tactical level with middle degree of abstraction.

Dynamic systems (DS) simulation is based on mathematical models of dynamic systems which consist of state variables and algebraic equations. These models are commonly used for physical systems with continuous behavior. DS is used on operational micro level with low degree abstraction. Examples are Finite Element Method (FEM) or Computational Fluid Dynamics (CDF) approaches.

Agent based (AB) simulation can be used to model the behavior of active agents in a defined environment. Each agent acts individually based on its implemented logic and interacts dynamically with other agents. The system behavior is determined in a decentralized manner without a global control.

System dynamics (SD) models describe the behavior of a corresponding system with a set of differential equations representing interacting feedback loops and flows affecting stock variables. SD is usually used on strategic level with high degree of abstraction.

Figure 2.10 structures these approaches according to their level of abstraction and discrete or continuous behavior. Borshchev and Filippov further explain in detail how these approaches can be combined to model a desired system behavior.

An important challenge in model development is determining the required detail of models. Very detailed models contain many objects and cause effort in development and maintenance. Very simplified models bear the risk of being too coarse and not sufficiently accurate for the given planning task (Rose and März 2011). Moreover, Sterman (2000) suggests to avoid black box models which do not provide

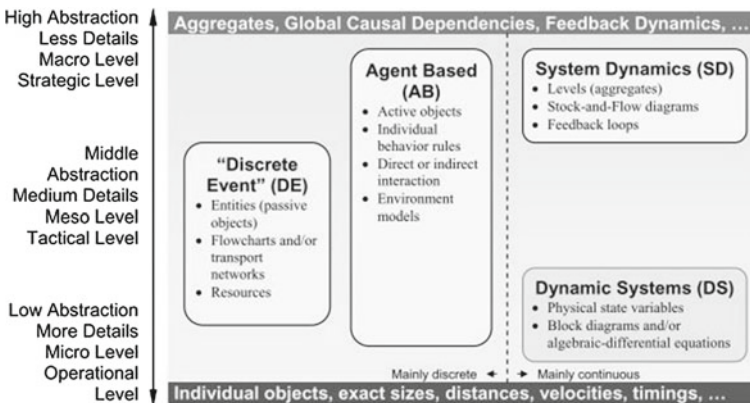


Fig. 2.10 Simulation approaches on abstraction level scale from Borshchev and Filippov (2004)

enough insight into the system behavior of interest. Other challenges are related to the clear definition of the simulation study objectives, the participation of all involved stakeholder, and availability of required know-how and skills, selecting of a suitable simulation tool, as well as sufficient validation (Wenzel et al. 2008). In order to support model developers and simulation engineers, different but similar procedure models were published for model development and simulation studies (Banks et al. 2010; VDI 2014; Rabe et al. 2008). The differences between these procedure models are mainly related to the complexity, scope and terms of the individual steps. Content wise, all models contain the steps related to objective analysis, model formulation, implementation, verification and validation, and employment.

2.2.3 *Simulation in Production*

Simulation is widely used in planning, analysis, and improvement of factories and the elements of production systems (Negahban and Smith 2014; März et al. 2011; Jahangirian et al. 2010; Schuh 2006). Entire production systems or material flows in process chains are usually represented by models which simulate the dynamic behavior of a system using a DE approach (Bergmann 2014; Rose and März 2011). According to the results of Jahangirian et al. 2010, DE and AB simulations were often used for scheduling, resource allocation, assembly line balancing, capacity planning, transportation and inventory management. In addition to DE and AB, SD approaches were used for strategic decisions such as supply chain management, project management, and organizational design. Moreover, simulation of process chains including DS process models is also seen to be beneficial for the improvement of product quality (Afazov 2013; Barthel et al. 2013). Such approach may allow a detailed analysis of the influences of processes on product characteristics. DS simulations are also usable for the detailed micro analysis of the interaction between processes and machines (Brecher et al. 2009). However, Afazov states that although simulation is often used for a macro-scale analysis of process chains, the micro-scale analysis of processes is still a challenge.

Already in 2004, Fowler suggested a real-time factory simulation which runs simultaneously to the real factory operation and instantaneously provides results for short-term decision making (Fowler 2004). Today this idea is for example addressed in the context of the Industry 4.0 initiative which aims at creating intelligent factories by using cyber-physical systems (CPS) consisting of virtual and physical elements as well as digital technologies such as augmented reality and internet of things (Kagermann et al. 2013). Similarly, the digital twin approach aims at combining a real world system with a virtual duplicate. This approach allows to understand how a product is transformed during production and also to trace the characteristics of a product throughout its life cycle (Grieves 2014). However, so far the most simulation applications focus on individual structural levels such as an entire production system, a production cell, machines and equipment, or processes (Landherr et al. 2013). In order to simulate an entire factory, new simulation approaches have to pursue a multiscale simulation of production systems with its structures and processes.

2.2.4 Multiscale Simulation

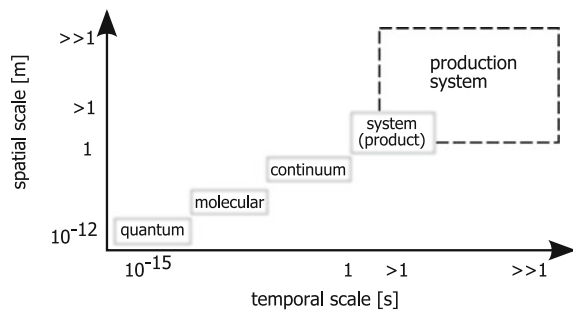
Many problems in science and engineering show multiscale solutions considering different spatial and temporal scales of individual systems or processes. The concept of multiscale modeling and simulation is established in various domains and disciplines such as biology (Boras et al. 2015), material science or “computational materials” (Wieser et al. 2015; McDowell and Olson 2009; Gates et al. 2005), or computational science (Hoekstra et al. 2007). The idea behind multiscale modeling is describing the behavior of one or multiple systems by separately considering different scales using the best suited methods and tools. As an example from material science, Gates et al. start a bottom-up approach by modeling at an atomic scale and by using molecular mechanics or dynamics methods. Next, moving up in scales from micro to meso scales using micro-mechanics until the system scale which can be analyzed with fundamental mechanics (Gates et al. 2005). Problems can be solved at particular scales and results can be passed to models addressing other scales. Thus, multiscale modeling allows bridging of scales.

Similar to physical or chemical systems, production systems can be observed at different spatial scales from unit processes over process chains and TBS up to the building. In addition, Bullinger et al. (2009) suggest to consider different time scales in production system simulation such as seconds, minutes, and hours or up to several years. For this reason, multiscale modeling and simulation is seen as a key feature in order to realistically imitate the operation of production systems (Landherr et al. 2013). Figure 2.11 illustrates how a production system may extend the commonly observed scales in multiscale modeling in both the temporal and spatial direction.

Production systems itself consist of system elements acting on different scales. These elements have to be modeled within a multiscale simulation based on the presented simulation approaches. Figure 2.12 presents a structure of simulation models for different scales considering different degrees of abstraction, simulation approaches, and model characteristics.

One risk related to detailed multiscale simulations is the high expected effort and required know-how for model development. This has to be considered since modeling effort, the required skill set of simulation experts, as well as the missing re-usability are common barriers of simulation which impedes the broad application

Fig. 2.11 Scales for the analysis of materials at nano scale and up to a production system; figure inspired by Gates et al. (2005) and McDowell and Olson (2009)



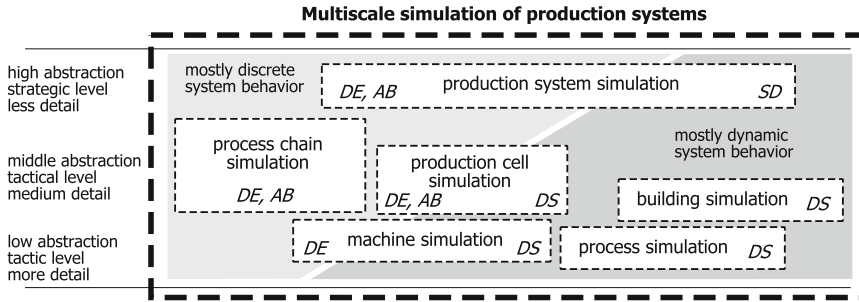


Fig. 2.12 Structure of simulation models for different scales considering suitable simulation approaches; figure inspired by Borshchev and Filippov (2004) and Landherr et al. (2013)

for production engineering (Bergmann 2014). Another challenge is the selection of suitable software tools for each production system element. Different tools exist for different simulation approaches and model characteristics. Typical software tools for DE simulation are Tecnomatix Plant Simulation (part of Siemens PLM software) or Arena. An established SD simulation tool is Vensim. The tool AnyLogic allows to combine DE, AB, and SD simulation. Established tools for DS simulation are Matlab/Simulink, Abaqus, Adams, or Dymola (Modelica). Consequently, the realization of multiscale simulations requires the combined application of different software tools or the complete implementation of all models within a multimethod simulation software such as AnyLogic.

These challenges are partially addressed in the digital factory by providing interfaces and workflows to connect existing models and to enable the re-use of models. Furthermore, it is suggested to develop separate models of different factory elements and to create seamless interactions between these models and used tools in order to achieve a distributed simulation model of a production system (Bullinger et al. 2009; Fowler 2004).

2.2.5 Co-Simulation

During the last decade, a new simulation paradigm evolved aiming at the coupling of different simulation models. The goal of coupled simulation or so-called co-simulation is the integrated analysis of system elements and their interrelations by coupling of multiple simulation models or tools for systems and sub-systems (Sweafford and Yoon 2013; Brecher et al. 2009; Zülch et al. 2002; McLean 2005). A clear and standardized definition of the term co-simulation has not yet been established (Geimer et al. 2006).

In co-simulation, each model represents a part of an entire system and exchanges data with other models during simulation runtime. Co-simulation is motivated by an increasing complexity of systems which requires an interdisciplinary collaboration of experts. Co-simulation allows to use the best suited simulation tools for each sub-system, to re-use models, to reduce the modeling time, and to represent a sub-system in greater details than it would be in a monolithic model (Sicklinger et al. 2014; McLean 2005). As a result, co-simulation may lead to a time-efficient execution of an entire system simulation and a high accuracy of simulation results (Aurich et al. 2009; McLean 2005). Examples of co-simulation applications are multi-physics problems (Sicklinger et al. 2014; Brecher et al. 2009; Errera et al. 2011), agent-based systems (Morvan et al. 2012), multi-level material analysis (Gates et al. 2005), building energy and control design (Zuo et al. 2014; Zhang et al. 2013), and planning of production systems (Pedrielli et al. 2011; Zülch et al. 2002).

The data exchange between different models is a great challenge with respect to accuracy and stability of the transfer and the results. Different strategies for coupling and synchronization were developed and evaluated (Sicklinger et al. 2014; Sweafford and Yoon 2013). The coupling of models can be realized by direct connections between simulation tools or via centralized middleware software (e.g. based on principles of High-Level Architecture (HLA)) (McLean 2005; Raab et al. 2008; Kossel et al. 2006). The task of middleware software is the synchronization of data exchange and communication between different simulation programs. Wetter (2010) developed the open-source middleware interface Building Control Virtual Test Bed (BCVTB) for coupling different tools such as EnergyPlus, Dymola (Modelica), Matlab and Simulink in order to allow an integrated building energy simulation (Wetter 2010; Wetter et al. 2011). Common applications of the BCVTB are in the context of building energy and control system evaluation. A commercial middleware solution is TISC which consists of a TISC server and different TISC clients for implementation in the coupled simulation tools (Kossel et al. 2006).

In co-simulation, models can be executed in a serial, parallel, or integrated configuration (Sweafford and Yoon 2013; Leobner et al. 2011) or with fix or variable time steps for data exchange. Sweafford and Yoon have shown that the parallel and integrated model executions provide identical results while the results of serial simulations differ (from the parallel configuration) and are less accurate. Furthermore, a serial configuration of multiple models results in longer execution times, especially if models with long execution times are involved and other models have to wait for the results. However, parallel coupling of models also cause challenges such as the combination of discrete and continuous models (Leobner et al. 2011).

The simulation of complex production systems can benefit from the combination of different modeling types, simulation approaches, and software tools. Co-simulation with specialized models of different production system elements or scales can improve the simulation results also for the simulation of battery production. Moreover, the combination of specialized models to a comprehensive multiscale model requires the investigation of interactions and the definition of interfaces, which fosters a deeper understanding of the observed system.

2.3 Summary and Preliminary Findings for the Simulation of Battery Production

Battery systems consist of different components which relate to different production stages each of which has specific requirements in production. Cell production is characterized by sequential process chains with specialized processes. These processes require comprehensive machines and equipment which is expensive and have partially very high energy demands. These processes – along with the used materials – have strong influences on the product quality. In addition, cell production makes great demands on the environmental ambient conditions such as temperatures, humidity and cleanness which requires specific building equipment. Additional TBS are needed for compressed air generation and air suction. Due to the expensive and comprehensive facility infrastructure, machines, and equipment, it is important to achieve high utilization and throughput in order to decrease specific production costs and environmental impacts for each cell unit.

The assembly of modules or systems is characterized by handling and assembly tasks which are relatively less complex compared to cell production. Furthermore, the requirements for building environment conditions are not as high compared to cell production. However, the product variety is much higher compared to the variety of electrodes or cells.² Consequently, it is a challenge to achieve a high production system utilization and short throughput times while dealing with high product variety. This demands for a flexible production system.

Simulation of production systems or factories is – in general – used for the analysis and improvement of the production activity and to support product development and production management. It is suggested to consider multiple scales of production systems and to use the best suited simulation approach for each production system element. The simulation of battery production – in particular – shall consider the production of all production stages from electrodes to systems. It should enable the evaluation of the production performance based on various indicators which allow the identification of hot-spots for improvement regarding quality, costs and environmental impacts. In this regard, relevant are the utilization of machines and the entire system, the lead times of jobs, the output of finished product units per time period, the material demands per product unit, quality rates or scrap, as well as the energy demands of machines and TBS equipment. Since different materials and energy carriers have different impacts, the simulation has to differentiate material types and energy carriers (e.g. electricity or gas). Moreover, while material demands and energy demands of machines correlate with the output of final products, the energy demands of peripheral equipment and TBS are independent of the output. Thus, it is of interest to determine the energy demands per product unit in addition to the overall energy demand.

To determine these indicators, the simulation has to imitate discrete unit processes considering the influences of processes on product characteristics, machine

²For example, modules and systems can be assembled by using different cell types, different quantities of cells, different housings, and with or without a cooling system.

behavior, as well as the related energy and materials demands. In addition, the material flow has to be simulated in order to determine the output and utilization of the production systems. The simulation must be able to imitate sequential process chains (cell production) as well as shop floor configurations allowing a flexible material flow (module and system assembly). Furthermore, the simulation must consider the influences of product variants on processes and the material flow.³

These relevant production system elements can be simulated by using different approaches. DE simulation is suitable for describing the material flow of product units between machines. An AB approach allows modeling of system elements as individual instances with specific properties and characteristics. This would enable to simulate the individual characteristics of product units and their development along a process chain. DS simulation approaches are suitable to imitate the behavior of dynamic systems such as machines, processes, or TBS equipment. The combined and parallel utilization of different simulation models enables to use the best suitable software tools for each sub-model, and to re-use existing specialized models of involved stakeholders.

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³For example, the material flow of electrodes and modules is completely different and the coating of a double sided electrode takes more time compared to a single sided electrode.

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