The International Journal of Advanced Manufacturing Technology (2019) 102:1373–1390
https://doi.org/10.1007/s00170-018-3054-y

ORIGINAL ARTICLE

Multiscale simulation approach for production systems

Application to the production of lithium-ion battery cells

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Received: 18 November 2017 / Accepted: 18 November 2018 / Published online: 7 January 2019

Abstract

Planning support for industrial production systems aims at reducing production-related costs and environmental impacts while creating required products with a desired quality. However, the increasing complexity of modern products and production technology makes planning and the provision of appropriate methods and tools a challenging task. Isolated measures for improving quality, cost or eco-efficiency, often result in problem shifting causing negative effects regarding other goal criteria. For this reason, suitable methods and tools are required for the planning and evaluation of specific improvement measures and for obtaining an interdisciplinary system understanding. This paper presents an approach, which is capable of analyzing production systems considering multiple scales based on coupled simulation models. The approach enables the evaluation of interactions between product units, processes, machines, technical building services, and the building structure. The approach contains a generic framework for the simulation structure, detailed model concepts for relevant production system elements, and a definition of interfaces between models for co-simulation. A case study demonstrates an exemplary application of the simulation approach for the production of battery cells. The study shows how the simulation enables evaluating the influences of different process configurations on intermediate product characteristics as well as of different factory scenarios and seasonal effects on the energy demands. More specifically, on product and process scale, the study revealed how different process routes and process parameters in electrode production affect the characteristics of battery slurries and coated electrode foils along with production lead-times. On process chain and factory scale, the study illustrates how the energy demands of machines and building services are influenced by machine operation and outside weather conditions. Thus, the study provides insight into the capabilities of a multiscale simulation and how such simulation may be applied to evaluate different producton system configurations, operation strategies, or facility locations.

Keywords Multiscale simulation · Model coupling · Co-simulation · Battery cell production

1 Introduction

Production is the major mechanism not only driving wealth in many countries [1] but also enabling the availability of key technologies for transforming the energy and mobility sector by providing products such as wind turbines, photovoltaic modules, and batteries for electric vehicles.

On the one hand, production leads to the creation of goods with demanded and innovative properties by using resources such as machines, energy, and materials. On the other hand, production causes various emissions to the environment such as carbon dioxide, noise, waste, or pollutants. Consequently, it is of interest to reduce production-related costs and to minimize environmental impacts while creating required products with a desired quality.

However, the improvement of production systems and products is a challenging task since manifold cause effect relationships can lead to problem shifting between different goal criteria within a production system or an entire value chain [2, 3]. This is in particular the case for the production

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of complex products—such as large-scale batteries—which consist of many different components and require various processes, diverse production equipment, or specialized factories. Well-intended improvement measures—such as adjusted process parameters, use of new materials, or new machines and tools—may result in local improvements but could also cause undesired effects on other production sectors, processes, product characteristics, or equipment (e.g., technical building services (TBS)), leading to reduced product quality, higher costs, or higher environmental impacts overall.

In order to improve production systems without causing problem shifting, production engineers and product designers must have an interdisciplinary system understanding. This includes knowledge about the interrelations between process parameters, used materials, product quality and properties, building ambient conditions, yield, production system utilization and bottlenecks, production strategies (e.g., batch or single product unit flow), TBS operation, and resulting material and energy flows. Such knowledge enables deliberating and evaluating the impacts of isolated improvement measures on an entire production system.

For attaining this knowledge and for analyzing the effects of planning and design decisions on a production system and the resulting products in an integrated manner, engineers and designers from different disciplines require methods and tools. Such methods and tools must support in gaining insight into the static and dynamic characteristics of production system elements as well as their interactions including the effects on resulting product properties. In this regard, one powerful and promising method is computer simulation. It is an established method in industry and research, which allows examining the behavior of complex dynamic systems. Many simulation concepts and applications can be found for different planning tasks and planning horizons as well as for selected individual structural levels of a production system such as an entire system, a production cell, machines and equipment, processes, or factory buildings (e.g., [4, 5]). However, simulation approaches allowing investigating the entire production systems including all relevant system elements and their interactions in detail are rare [6]. Moreover, the required know-how and high effort related to the development, employment, and maintenance of simulation models is a barrier to the broad application of production simulation in industrial planning practice [7]. Consequently, there is the need for a simulation approach, which allows imitating complete production systems holistically, considering different scales [8] while been manageable and applicable within industrial planning processes.

This paper presents a multiscale simulation concept, which includes the relevant characteristics and elements of production systems required for an integrated evaluation of improvement measures regarding economic, environmental, and technological goals. The main principle of a multiscale simulation is the modeling of system elements on different temporal and spatial scales and the exchange of the generated results between scales during simulation runs. An example: a production machine or process can be modeled in detail considering the behavior of individual components precisely for time periods of seconds, minutes, or hours. The operation and utilization of the machine is determined on a larger scale on process chain level depending on the production program defined for days, weeks, or months. The influence of heat emissions from machines and outside weather conditions on the energy demand of factory building heating or cooling can be evaluated for larger time periods such as months or years. Such multiscale simulations can provide insight into the system dynamics of a production system and support the holistic evaluation of improvement measures.

The remainder of this paper provides theoretical background about multiscale modeling and simulation as well as the relevant state of research, describes the developed simulation concept, presents an implemented simulation core model as the basis for specific simulation applications, and demonstrates the application and advantages of the concept within a case study exemplary for the production of lithium-ion battery cells.

2 Background

2.1 Simulation for production

Simulation is the imitation of an existing or planned real-world system over time based on a model. There are different simulation model types (deterministic/stochastic, discrete/continuous, static/dynamic), approaches (discrete event (DE), dynamic systems (DS), agent-based (AB), system dynamics (SD)), and software tools which have to be selected or combined with a specific simulation goal in mind [9, 10].

In production context, different types of simulation models and approaches are used depending on the scope and task of a simulation [5, 9, 11]. For example, detailed machine and process models use DS simulation, which are based on mathematical models to describe continuous state variables of a system. Material flows in discrete process chains are usually represented by DE models, which change the state of a system only at events and discrete points in time. Production planning tasks (e.g., resource allocation or assembly line balancing) are often supported by AB simulations which describe the interactions of decentralized individual units (agents) such as products or resources. Supply chain management often utilizes AB or

SD simulation to analyze dynamics of supply, demand and inventories with a higher level of abstraction. Furthermore, simulation approaches can also be combined in order to consider different system behaviors within one model or to assemble models for multiple systems. For example, the combination of a DE process chain model with DS process models enables assessing the production performance and resulting product characteristics in more detail (e.g., [12]). In process industries (e.g., chemical or pharmaceutical industries), DS simulation (flowsheet simulation) is widely used to simulate separation and transformation processes with continuous material and energy flows [13, 14]. However, since modern technologies, such as batteries, require discrete and continuous production processes, the border between process and discrete production industries becomes blurry.

The combination of models for all elements of a production system including product units within one simulation would enable analyzing dependencies between the involved system elements and the effects of local improvement measures on the overall system. Moreover, a real-time simulation of the entire factories could run simultaneously to the real production operation and immediately provide results for short-term decision-making [15]. However, most simulation applications aim at isolated production system elements (e.g., processes, machines and equipment, process chains). In order to simulate an entire production system and to realize an integrated evaluation of improvement measures, innovative simulation approaches must pursue a multiscale perspective considering all structures and processes.

2.2 Multiscale production simulation

Multiscale modeling and simulation is an established method in many disciplines such as material science (e.g., [16, 17]), computer science (e.g., [18]), and biology (e.g., [19]). Its basic idea is replicating the behavior of a system by separately modeling different scales, each by using the most suitable methods and tools. In the same way as for materials and other physical or chemical systems, production systems can be observed at different spatial and temporal scales. Spatial scales range from unit processes over process chains and TBS up to the building (e.g., [20–23]), all of which can be analyzed for periods (temporal scales) such as seconds, minutes, and hours or up to several years (e.g., [8]). Figure 1 sets scales for a production system in perspective relative to commonly used scales for multiscale analysis.

The elements of a production system and their behavior can be simulated in different ways. Figure 2 presents a structure of simulation classes for different production system elements with respect to the degree of abstraction and level of detail, simulation approaches, and model characteristics.

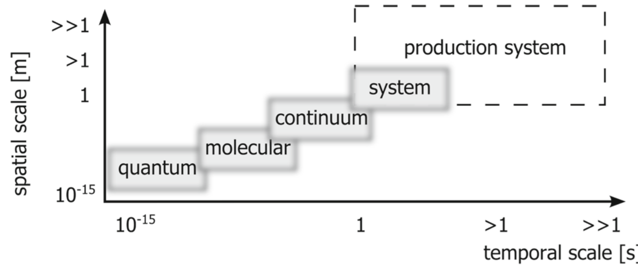


Fig. 1 Common scales for multiscale material analysis extended by manufacturing system; according to [6], inspired by [17, 24, 25]

Various simulation approaches exist combining different scales of a production system. The concept Integrated Computational Materials Engineering (ICME) refers to modeling and simulation approaches which focus on the behavior and structure of materials as well as the effects of their processing (e.g., [26–28]). In the research field of Process Machine Interaction (PMI), simulation is used for analyzing interactions between processes and related machine tools such as impacts of vibrations or temperature on process stability and product quality [29, 30]. Related approaches consider machine structures along with process physics and the interaction with a product unit. Other approaches address the evaluation of energy demands of machine tools by combining simulation models for machine components and processes [31, 32]. On a larger scale, there are approaches, which combine multiple detailed models for machines or processes in order to determine the energy demand [33, 34] or the effects of process on product properties [12, 35] within the entire process chains. Combined models for process chains are also utilized for resource allocation and job scheduling with respect to economic criteria such as resource utilization or lead and delivery times (e.g., [36]). Similarly, combined models describing machines and processes including specific material flows are created to generate data for life cycle assessment studies in order to evaluate the environmental impacts of production [37, 38]. Detailed process chain simulations have also been further extended towards larger

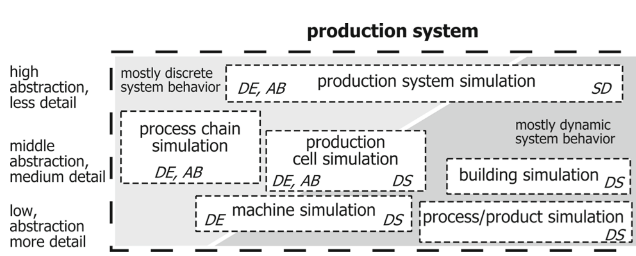


Fig. 2 Structure of simulation models for different manufacturing system elements; figure adapted from [6] and inspired by [10] and [4]

scales considering TBS and peripheral auxiliary equipment. This allows to determine indirect energy demands based on production operation as well as to derive energy efficient production schedules and hot spots for improvement within a production system (e.g., [39–41]) or product designs [42]. On an even larger scale, building simulation models are used in combination with machine and TBS models to study the effects of machine operation such as heat emissions and weather conditions of different factory locations on the energy efficiency of manufacturing systems (project ENOPA [43], project INFO (e.g., [44–48]), project THERM [49, 50]). Simulation for buildings has their origin in the context of building engineering, where various multiscale simulation approaches have been developed addressing the interactions between the building structures, HVAC systems and the operations (e.g., heat emissions of equipment or humans) within building zones (e.g., [51, 52]). A detailed discussion of the state of research in multiscale production simulation is presented in [6] and [39].

The actual combination of simulation models for production system elements can be realized by using different model integration or coupling strategies. Often, models can be integrated within other models or are implemented in the same software tool in order to avoid or reduce the effort of model connection. Models can also be implemented within different software and directly connected to share results after model execution or during simulation runs. Additionally, especially if different software tools are used for multiple models, coordinating middleware software can be used to synchronize the execution and data exchange between models within a co-simulation. However, despite allowing the use of the most suitable software tool for each model, co-simulation is seldom used and mostly utilized in simulations addressing small or large scales of production systems (process and machine interaction or building energy simulation).

2.3 Summary and research demand

The review of existing simulation approaches and publications revealed that there is a broad spectrum of simulation concepts and applications addressing different planning tasks and production scales. The idea of multiscale production simulation provides various advantages for the planning and improvement of production systems. However, no identified simulation approach considers all scales of a production system. Existing simulation models combining models for TBS and building structures with models for production operations mostly simplify the product, process, and machine scales. Also, simulations addressing process physics and product characteristics as well as traditional production objectives within a process chain usually do not include interactions with the building environment or TBS. Moreover, no found approach supports multiple planning perspectives and the evaluation of technological, economic, and environmental objectives in an integrated manner.

Table 1 summarizes the comparison of research contributions regarding the addressed scales, the use of co-simulation, and the contribution to the methodology of multiscale simulation. The table shows that no presented simulation approach is capable to represent all scales of a production system which would be required to achieve a holistic evaluation of multiple planning perspectives. Furthermore, only a few contributions utilize co-simulation or model coupling to connect models for different scale. And only very few contributions provide methodological guidance towards the development of multiscale simulations.

Consequently, there is the need for a new simulation approach which enables the development of holistic multiscale production system simulations which support multiple planning perspectives while considering all scales of a production system. The new concept must address the following main research demands:

- A process chain model must be developed as the core of a multiscale production simulation to define specific operational schedules as a basis for the determination of utilization, energy and media demands, TBS operation, and effects on building ambient condition. The model must allow to derive throughput times and yield of jobs or individual product units, aggregated energy demands, as well as costs for machining and used materials. This is needed for the evaluation of economic objectives.
- The process chain model must allow to include specific detailed machine models to enable the evaluation of influences of machine parameters or configurations on performance indicators on system level.
- Product quality and characteristics must be considered in order to evaluate technological objectives. Process models need to describe the impacts of processes on characteristics of individual product units considering relevant influences such as disturbances from machines, product type-specific process parameters, and ambient conditions.
- A new framework must define a modular multiscale production model structure with clear interfaces between sub-models which allows to add or exchange sub-models in order to achieve simulation results for operational, tactical, or strategic planning tasks. Whereas at an early planning stage, models and simulation results can be of less detailed character, specific operational decisions may require more accurate results in high resolution.

Table 1 Summary of research contributions (Harvey Balls indicate the degree of the consideration of production system scales and the use of co-simulation and of a methodological contribution)

Contribution	Scales						Co-simulation	Methodology
	Product	Process	Machine	Process chain	TBS	Building	Model coupling	
Brecher et al. [29, 30]	◑	●	○	○	○	○	◕	○
Abele et al. [31]	◔	◑	●	○	○	○	◔	○
Eisele [32]	◔	◑	●	○	○	○	◔	○
Schrems [33]	○	◔	●	◑	○	○	◔	○
Weinert [34]	○	○	●	◑	○	○	○	○
Liang [12]	◔	◑	◕	◕	○	○	◕	○
Colledani [35]	●	●	◑	◔	○	○	◔	◔
Cho [36]	◔	○	◔	◑	○	○	◔	○
Heilala et al. [37]	◔	◔	◔	◕	○	○	○	○
Sproedt [38]	◔	◔	◑	◕	◑	○	○	○
Seow and Rahimifard [42]	◑	◔	◕	◑	◕	◔	○	○
Thiede et al. [39, 40]	○	○	◕	●	●	○	◕	○
ENOPA (e.g., [43])	○	○	●	●	●	●	◑	◔
INFO (e.g., [44, 45])	○	◔	◕	◔	◕	●	●	◕
Bleicher et al. [48]	○	◔	◕	◔	◕	◕	●	◑
THERM (e.g., [49])	○	◔	◑	◑	◕	◕	○	○
Wetter (e.g.,[52])	○	○	○	○	●	●	●	◕

3 Concept

The purpose of a multiscale simulation for production systems is supporting an integrated planning and evaluation of improvement measures regarding product quality, production costs, and environmental impacts, as well as supporting the generation of an interdisciplinary system understanding. It shall foster the cooperation of experts from different planning disciplines by combining their expertise and knowledge into one holistic approach.

Figure 3 shows how the disciplines involved in the development and improvement of a production system can utilize a multiscale simulation in order to evaluate specific improvement measures virtually and to generate results indicating the potential impacts on production system level.

The integration of specialized simulation models into a multiscale simulation requires the definition of specific inputs and outputs considering each scale. For this purpose, the concept provides a fundamental structure, which is flexibly adaptable to different production system configurations and product types. This includes the description of system boundaries, a framework for relevant system elements, and specific model concepts for their behavior and interactions.

3.1 Framework

The generic framework, shown in Fig. 4, structures production system elements into simulation sub-models and proposes interfaces between these sub-models to ensure

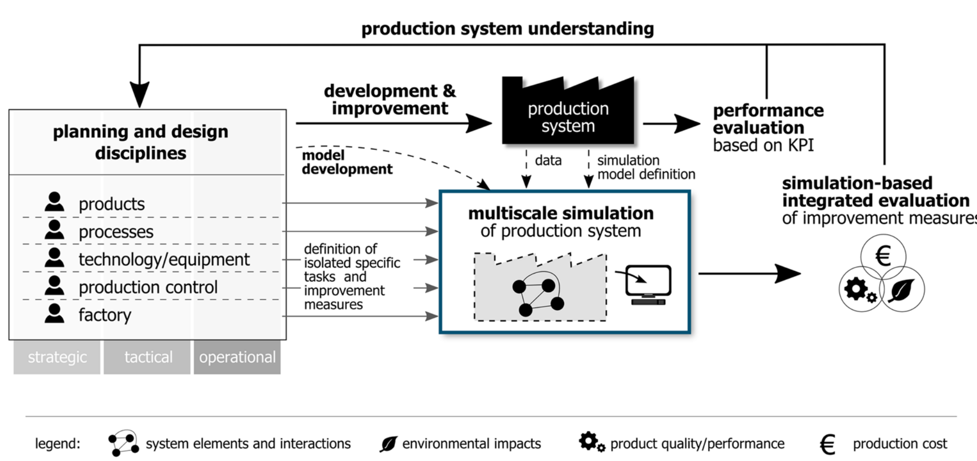


Fig. 3 Scheme of a multiscale simulation of battery production systems; based on [6]

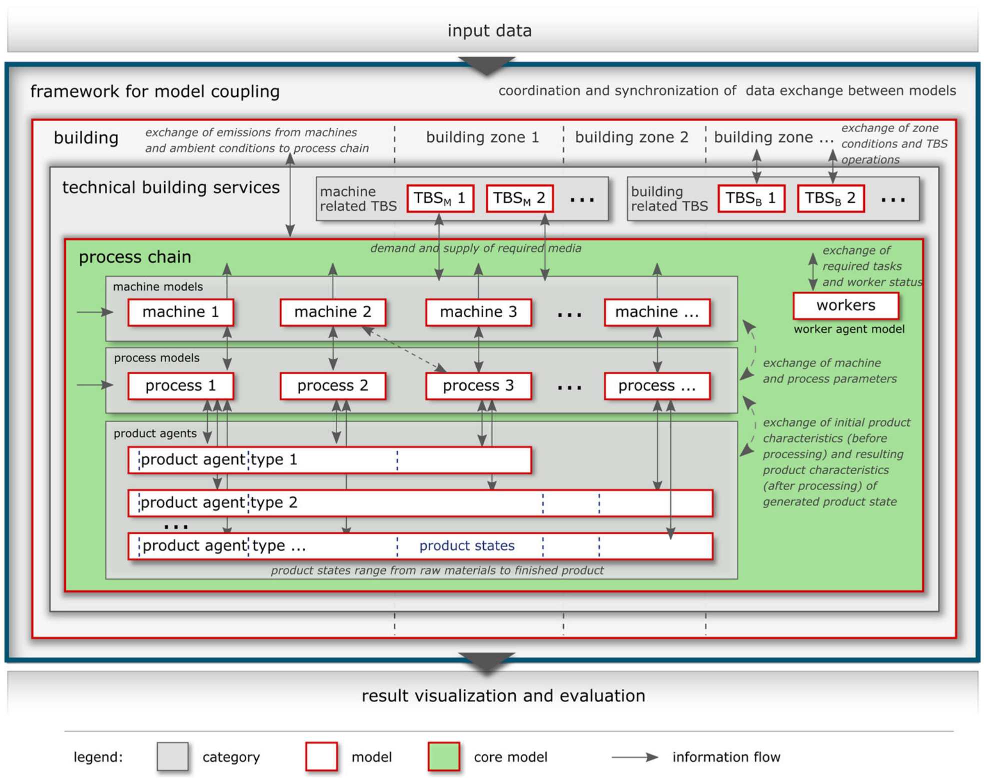


Fig. 4 Framework for multiscale simulation of manufacturing systems; based on [6]

a lean information flow. It is based on the hierarchical structure of production systems considering spatial and temporal scales. The framework is assembled from layered simulation model categories, exemplary model instances, and generic potential flows of information.

The first upper layer contains models for individual machines, related processes, and products of different product types as well as individual workers. The elements of the first layer are part of a process chain (2nd layer) of which the operation defines the activity of each individual element. These elements of a process chain enable describing dynamic aspects such as the material flow of product units between processes, the modification of product characteristics within processes, and production resource utilization. Since a process chain model has to have interfaces to most other models, it can act as a core model which aggregates information and coordinates the information flows between models on different scales. The operation of process chains and factories requires different TBS. These TBS can be differentiated between machine-related services (TBS_M, e.g., compressed air supply) and building-related services (TBS_B, e.g., air conditioning, lighting). Thus, TBS are on a larger scale compared to machines but on a smaller scale compared to the building. For simplification, machine-specific TBS (e.g., air suction) are part of related machine models. A process chains with its elements and TBS are located within a factory building, which forms the lowest model layer of the framework. All sub-models are embedded within a simulation infrastructure which serves for model coupling and provides mechanisms for data exchange and synchronization of sub-models. This also includes interfaces to required data sources (e.g., energy demand data of machines or building construction data) and for the export of simulation results. A the derivation of the framework regarding the definition of system boundaries, hierarchy, and scales as well as of the sub-model concepts is described in [6].

3.2 Sub-models

The sub-models representing individual production system elements must provide specific functionality, results, as well as defined inputs and outputs in order to enhance and to interact within a multiscale production simulation. The inherent logic of each sub-model must be developed for each particular system element but there are generic considerations as guidance for their development. The following paragraphs summarize the proposed formal descriptions of sub-models for process chains, machines, processes, and products, as well as TBS and buildings.

3.2.1 Process chain

The purpose of a process chain model is the representation of material flows and the related timing of machine operations in order to derive performance indicators such as utilization or lead times and to gain insight into bottlenecks or non-productive timeshares.

Process chain elements and material flow The model must allow the specification of a process chain, which consists of a number (MN) of machines or workstations, each with a buffer (B). A process chain can produce a number (PTN) of different product types (PT), each of which needs a finite sequence of production steps (PS). These steps indicate the order of required processes for each product type and each step must be assigned to (at least) one machine. This allocation and the order of production steps determine the possible routing of product units. However, the material flow (MF) of product units differs for single unit or batch production strategies. Single unit flow means that a single product unit of an associated job (J) moves to the next suitable machine as soon as it is finished with processing. Batch production means that all product units of a job are processed simultaneously on a machine or are buffered before moving to the next machine until all units are finished with processing. In this second case, all or many product units of a job move between machines at once. Since the accurate modeling of single unit or batch processing is important to determine the utilization of machines and the material flows, the process chain model must allow simulating both types of processing. For this purpose, the concept of processing units (PU) is introduced. A processing unit may represent a single product unit or a batch and they are the entities in the model which are processed within a machine and which move between machines during simulation. Consequently, a job can consist of one processing unit (one batch or single product unit) or multiple processing units (multiple product units). This model feature enables a flexible configuration of different process chains and job types as well as to define converging and diverging material flows. Figure 5 shows a schematic of the process chain elements within a shop floor coordinate system. The same logic is also usable for the representation of continuous processes. In such case, multiple machines can be directly linked, representing different stages of a continuous production facility, and product units represent fractions of a continuous product stream.

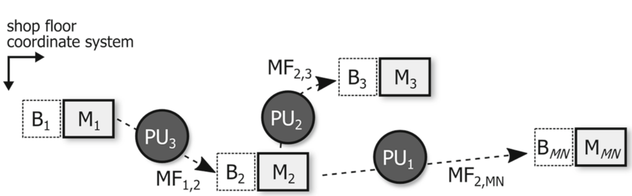


Fig. 5 Process chain structure with machines (M), buffers (B), material flows (MF), and processing units (PU), according to [6]

In addition, human workers can be included within a process chain as agents with individual skills, machine allocation, movement paths, and work intensity levels.

Configuration and control strategies A flexible model structure should allow to model different process chain configurations such as sequential production lines for similar products or layouts for flexible and agile production for a multiple product types. An example of a configuration for agile production is the so-called matrix-production, in which machines offer multiple and different production capabilities and the allocation of product units to machines is not predetermined. This avoids a fixed tact time and aims at increasing the utilization of a process chain while facing high product variety and uncertain demands [53, 54]. Such configuration highlights the importance of a flexible model structure, which can be based on individual machine and product agents. Machine agents provide the processing capabilities, which can be requested by product agents, which select the most suitable machines [53, 55]. The selection of machines for processing units can be either centralized with a global production control strategy (e.g., aiming at high utilization) or decentralized with specific decision rules and criteria for each individual processing unit agent (e.g., shortest lead time). The control algorithms within the process chain model require input information from machine agents to consider operational states and the availability of machines. The agent-based approach enables to replicate existing process chains as realistic as possible and also to model innovative process chain configurations.

Energy flows The determination of energy demands is necessary for the evaluation of energy costs and environmental impacts. The central character of the process chain models within the multiscale simulation facilitates the representation and aggregation of energy demands and flows of and between various production system elements. Figure 6 shows exemplary energy flows within a production system.

The process chain model can determine the overall energy demand by considering the power demands of machines and TBS over time, which directly depend on the

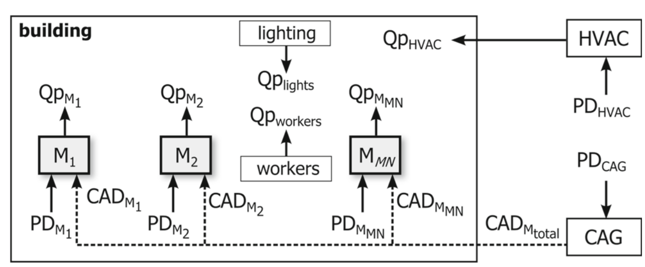


Fig. 6 Exemplary energy flows during production operation (PD: electrical power demand, CAD: compressed air demand, CAG: compressed air generation, Qp: heat flow)

production operation. Examples of relevant TBS systems are compressed air generation, lighting, and HVAC. The power demands of compressed air generation and HVAC depend on operational factors such as the aggregated compressed air demand of all machines or the heat emissions (of machines, lights, or humans) to the building environment. The specific power demands of machines and TBS systems must be determined in specific detailed models and communicated to the process chain model for the overall evaluation. Within the process chain model, is also possible to identify non-productive timeshares and energy demands as well as to allocate the direct and indirect energy demands to individual product units (embodied energy).

Production costs Besides the energy demand, relevant factors for the calculation of production costs are the utilization of the process chain as well as costs for machining, inventory, labor, and used materials. The process chain model can determine the utilization and inventory levels based on operational states of machines and the defined processing times for each product type and production step. The agent-based approach allows assigning material demands to processing units in order to perform a dynamic material flow cost accounting. Likewise, machining costs (based on a machine hour rate) can be assigned to a product unit depending on the time spent on a machine. Moreover, if workers are considered within the process chain model, it is possible to determine how many workers are required to operate the given set of machines and equipment. In addition, the model allows determining the achievable output of product units per time-period in order to allocate indirect costs (e.g., overall cost of TBS) to all finished product units.

3.2.2 Machines

Machine models describe the behavior of machines within a process chain along with the related energy and media demand profiles and heat emissions. Machine models can be realized with different levels of detail. For the use in the multiscale simulation, machine models must at least be able to represent generic operational states of a machine (e.g., on, idle, processing), relevant parameters, and characteristics associated with these states (power and compressed air demand, heat emissions), as well as the transition conditions between these states (e.g., ramped-up, processing finished) and overall failure behavior (e.g., probability distributions for mean time to failure (MTTF) and repair (MTTR)); similar for example to [34, 40]. Whereas the determination of electrical power demand and compressed air demand is mostly accurate enough as a discrete average value for each operational state resulting in a demand profile, heat emissions must be calculated continuously since a warm machine emits heat also when it is already turned off or to idle state [43].

3.2.3 Products and processes

Each processing unit (product agent) contains a sub-model, which stores and provides information about the product type-specific required production steps, processes, and related product specifications. Moreover, the agent describes the evolution of product characteristics and tracks the progress of production along a process chain. Each product type is characterized by a specific set of product characteristics C (C = 1, ..., C_{NPC}) which are transformed along the production steps. During production, each processing unit can be in different states of which state 0 describes the state prior to production and the last state NPS refers to the finished product. Figure 7 illustrates a product agent with generic product states and how characteristics can be transformed or created.

If multiple processing units have been assembled into the product characteristics have to be transferred and combined within the absorbing processing unit. Similarly, if a processing unit is divided into multiple units, the characteristics have to be assigned to all units accordingly.

The specific creation pr transformation of product characteristics is defined within separate sub-models. For each process, process models describe the resulting characteristics based on various influencing factors such as process parameters, already existing product characteristics, environmental conditions, machine tolerances and disturbances, or material properties. A process model must be connected to a related machine model to provide required machining parameters and to get inputs about disturbances and other influences on the processing results. Moreover, a process model must connect to product agents to receive existing product characteristics as an input and to provide the resulting product characteristics to the next product state. Figure 8 shows the integration and interaction of product agents and process models.

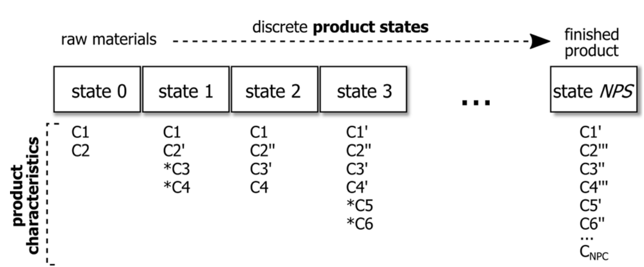


Fig. 7 Product agent with discrete product states and product characteristics (*: created; ': modified)

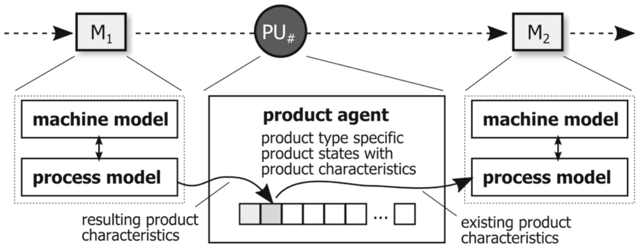


Fig. 8 Interaction of process and product models within process chain structure

Process models can represent processing tolerances and deviations of the processing results for each productions step. This enables observing the impacts of adjusted process parameters or modified machine tolerances on product quality and related economic aspects (e.g., higher/lower yield). In addition, the agent-based structure allows the tracking of product characteristics and thus analyzing amplifying or damping effects of process tolerances on specific product characteristics along entire process chains. In this regard, three different types of variation of product characteristics play an important role. First, processing results for product characteristics can vary for different processing units (e.g., processing unit PU_1 has a different value for product characteristic C_4 (e.g., weight) than PU_2, although both are of the same product type). Second, a product characteristic can vary within one processing unit (e.g., the coating thickness of a surface is not constant for one processing unit) but this variation is similar to all processing units of the same type. Third, variations of a product characteristic occur within a processing unit and between processing units. Figure 9 illustrates the types of variation.

Variations of resulting product characteristics within a process can be modeled by using probability functions, which have to be determined by theoretical considerations or empirical data. Distributions are characterized by the location of an expected value along with the a spread and shape of the probability function. Since product agents provide information about existing product characteristics, the simulation is able to evaluate the effects of these existing characteristics on the variations. Three different scenarios should be considered in the modeling of variations: First, the variation of one characteristic within a process is described by a defined probability function. Second, the spread and shape of the distribution depends on already existing product characteristics. Third, existing characteristics influence the expected value as well as the spread and shape of the probability function for a resulting characteristic. These three types of effects are illustrated in Fig. 10.

Different types of process models can be used depending on the available process knowledge. Examples of model types are deterministic or empirical parameter models, empirical stochastic mathematical models, and numerical models based on process physics. In addition, physical and empirical models can also be combined, as for example shown for the modeling of grinding processes [56].

3.2.4 Technical building services

Relevant TBS systems, which should be included within a multiscale simulation, are compressed air generation (CAG), HVAC, and lighting.

Compressed air generation Compressed air is generated in compressors, stored within a tank, and provided to machines or equipment via a system of pipes and valves. In addition, CAG systems may utilize filters or other air treatment devices. The pressure within the CAG system has to be kept stable within a defined range. This is realized with specific configurations of compressors according to control strategies. A model (typically a numerical DS simulation) can determine the system pressure and the energy demands for CAG depending on the total compressed air demand provided by the process chain model (similar to [40, 57]).

HVAC Depending on specific requirements for inside ambient conditions, building zones must be ventilated and the air may have to be cooled, heated, or dehumidified (air conditioning). For these purposes, the so-called air handling units (AHU) are installed. Specific AHU may be required for dry or clean room conditions. Simulation models of

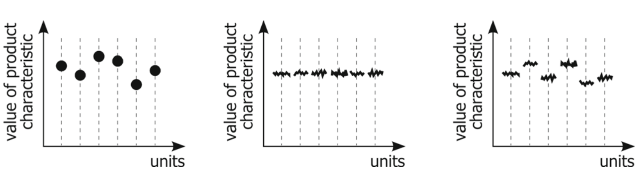


Fig. 9 Types of variation for a product characteristic: between different processing units (left), within processing units (middle), within and between processing units (right)

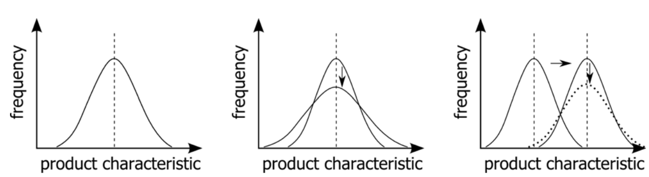


Fig. 10 Effects of existing product characteristics on process results: Product characteristic depends only on probability (left), existing characteristics influence distribution (middle), existing characteristics influence expected value and distribution (right)

HVAC equipment or AHU should determine the required operation and related energy demands depending on desired ambient conditions.

Lighting Building zones must be enlightened during production operation and different areas may have specific requirements regarding lighting intensity. In addition, light sources can be of different type, efficiency, and lifetime. These factors influence the overall cost and energy demands of lighting. It is of interest to determine the duration of usage per building zone as well as the energy demands.

3.2.5 Building

A factory building is usually divided into several building zones which are characterized by different thermal behavior and ambient condition requirements (e.g., regarding temperature, cleanness, humidity). A building simulation (typically based on physical numerical models) enables determining the indoor ambient conditions considering the building construction (e.g., ground plan, number of floors or windows, used materials) as well as internal (e.g., heat emissions depending on production operation) and external (e.g., weather conditions based on location) influences. In contrast to static calculations of extreme thermal conditions within building zones, which are suitable for the design of HVAC systems, simulations must continuously determine the ambient conditions to derive the specific operations of HVAC systems over time. Different existing building simulation tools can be used for this purpose [58].

3.3 Model connection and coupling

The various models must be connected to exchange information during run-time of the multiscale simulation. This requires a definition of interfaces between models and the selection of strategies for synchronization and information exchange. A standardized set of interfaces between model classes allows the practical re-use of existing models in the larger context of a multiscale simulation, which results in a reduced effort for model development. This

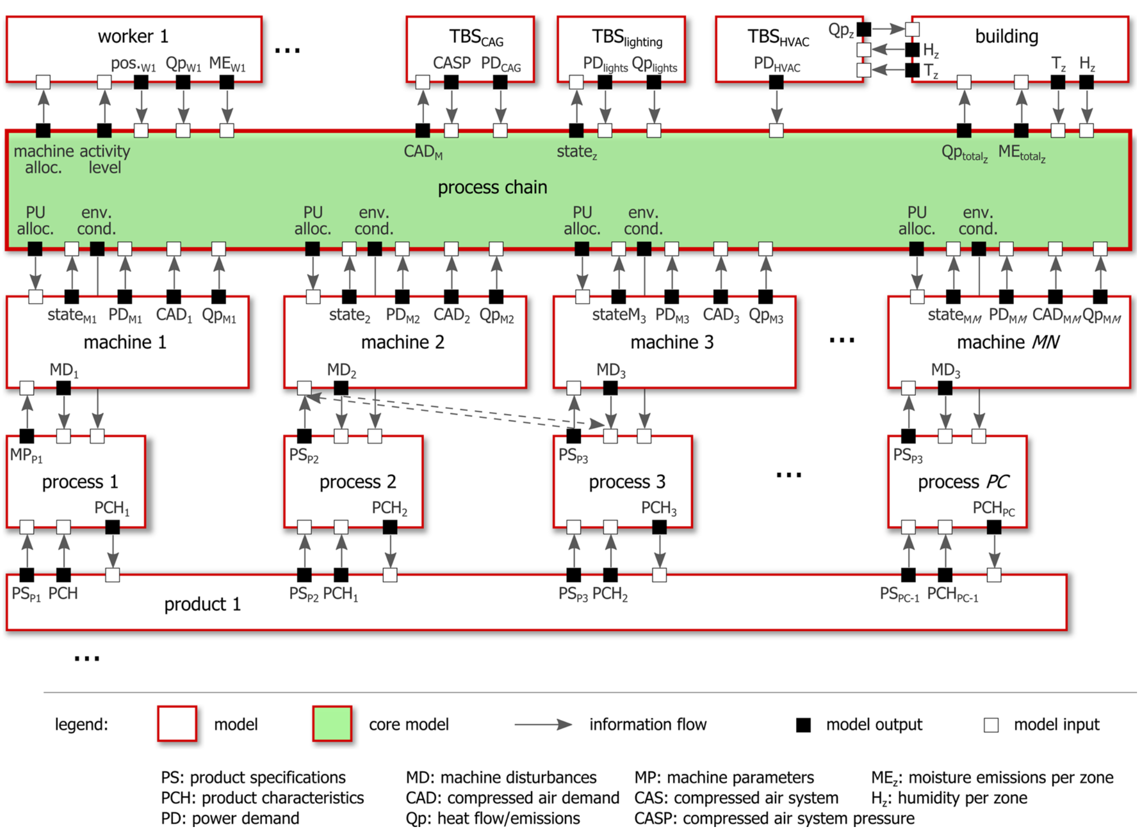


Fig. 11 Structure and exchanged variables of total multiscale model [6]

is in particular relevant for the collaboration of different planning disciplines, which use specialized simulation models.

Figure 11 illustrates generic interfaces between the exemplary model instances according to the previously defined framework.

The information flows between the models are indicated as output and input variables (output ■ → □ input). A product agent provides specifications and existing product characteristics to process models. Process models provide required machine parameters to machine models and receive information about machine disturbances. They also describe the modification of product characteristics, which are stored in the respective product agent. Machine models communicate their operational states, power, and compressed air demands, as well as heat emissions to the process chain model. The process chain level coordinates the activity of workers, forwards the total compressed air demand to the CAG model and the total heat emissions to the building model, sets signals for the lighting operation, and aggregates all energy and material demands for later result evaluation. The building model provides information about the ambient conditions for each zone to the HVAC model as well as to process models—through the process chain model—which consider environmental conditions within the determination of resulting product characteristics. The HVAC model returns information about the HVAC operation to the building model and provides the power demand to the process chain model. The connection of models within a multiscale simulation environment can be realized by different coupling concepts such as offline or direct coupling, model integration or co-simulation, which are shown in Fig. 12.

Offline coupling is only usable if there are two or few models and no parallel effects have to be considered, since simulation results of one model are only available after model execution. Model integration is suitable if models can be implemented within the same software. As an example, models of machines and TBS systems are integrated within a process chain model (e.g., [40, 42]). This avoids issues resulting from model synchronization since the same simulation time is used. Direct coupling of models

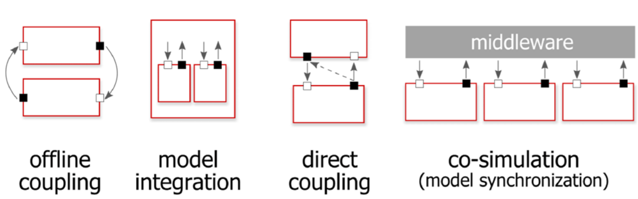


Fig. 12 Concepts for the connection of models [6, 39]

during runtime may be feasible if only few software tools have to be connected and one model can act as a coordinator. An example is the connection of a numeric process model to a machine model. The machine model can call the process model, pause, and resume after the process model has determined the resulting product characteristics of the processed product unit. Co-simulation using a coordinating middleware software is reasonable if multiple software tools have to be connected (e.g., a DE simulation tool for a process chain model and a DS simulation tool for a process or building simulation) [6].

3.4 Result evaluation

The generated simulation results enable gaining insight into cause-effect relationships between the modeled elements of a production system on different scales. For that purpose, the large amount of data resulting from the connected simulation models has to be processed to specific key performance indicators. These indicators should describe the overall performance of a production system as well as the performance and behavior of system elements. Since individual system elements may have very different relevant criteria and requirements regarding result resolution, an overall evaluation also requires aggregated indicators on larger scales. As an example, the overall energy demand of a production system must be determined by summing up the energy demands of all machines and TBS systems. Moreover, on system level, the total material consumption—divided into raw and auxiliary materials—can be determined by the material demands of each process. Considering different energy carriers and material types allows calculating the environmental impacts from energy usage (e.g., regarding global warming potential in equivalent CO_2 emissions). The total energy and material demand can be allocated to the number of finished product units in order to determine the specific demands. Each job and product unit can be characterized by a lead-time as well as value adding and non-value adding timeshares and specific energy demands. Moreover, the simulation enables to generate dynamic value stream representations for each product unit, job, or product type, which allow evaluating bottlenecks and hot spots. Such representation is just an example of how simulation results can be visualized for decision makers from different planning disciplines.

3.5 Model validation

The validation of simulation models is an important step within model development. An estabished method for the validation of simulation results is the comparison with historical data. However, for multiscale simulations of the entire production systems, the amount of historical data required for a sufficient validation of the entire model would be very large and hard to acquire. Moreover, the validation can be challenging due to the large number of interactions and interdependencies between the simulated variables. For these reasons, it is necessary to perform a solid validation for individual sub models and each interface between models. A helpful technique in this context is a sensitivity analysis combined with extreme value tests. This clarifies how results of sub-models change based on the range of possible input values generated from other models.

4 Application for battery cell production

Battery cells are the core technology for future electric vehicles. Moreover, the production costs of a battery system can take up to 40% of the total production cost of a vehicle [59], which makes batteries a significant cost driver. And whereas about 75% of the battery cell costs are determined by the utilized materials, about 25% of the cost results from cell production [60]. Also, Yuan et al. report that about 30 GJ of the energy demand for the production of a battery cell (the so-called embodied energy) result from raw material production whereas about 60 GJ are related to the actual cell production [14]. These numbers must be improved while increasing the production capacity of battery cells fulfilling the growing global demand. Väyrynen and Salminen have calculated that an annual production capacity of 10^6 electric vehicles would require 10 battery cell factories which a production capacity of 3 GWh each [13]. Consequently, there will be a growing global production capacity as well as strong global competition within the battery cell market. Thus, it is of great importance to increase the efficiency of cell production facilities. This case study shows how a multiscale simulation approach can be applied to such production system.

4.1 Model environment

The exemplary simulation is centered on a process chain core model, which represents the shop floor operation of the observed lab-scale facility. It contains models for machines and processes, products, workers, and lighting; it defines the building zones according to a ground floor plan; and it provides interfaces to a CAG model and a combined HVAC and building model. A middleware software (TISC Suite) is used to couple the models. Figure 13 shows the model structure of the simulation environment.

The process chain model is developed within the software AnyLogic, which is a multi-method simulation environment. Inside the model, classes for machines, products,

Fig. 13 Model structure for exemplary simulation: A process chain core model is connected with a compressed air generation system model (CAG) and a building model by using a middleware software

and workers are implemented as populations of agents. Machines are located in the shop floor layout and product units and workers can freely move within the different building zones. Each agent contains the relevant logic and stores parameters and variables to represent individual characteristics. This enables to model specific machine properties based on a generic schema and to integrate process models into machine models. The CAG model receives the total compressed air demand and determines the compressor operation along with the resulting power demand profile. The model provides the system pressure and power demand. The model for the HVAC system and the building is realized in the software Simulink based on the International building physics toolbox (IBPT). Weather information is prepared from TRY-files for Germany. For validation purpose, some sub-models of this multiscale simulations, such as individual machine models, have been validated based on available production data from the observed lab facility. However, since not all model elements could be validated based on historical data due to the lack of sufficient data sets, many sub-models have been verified and validated via plausibility checks and sensitivity analyses. For this reason, this study serves as a demonstration of the principles of a multiscale simulation rather than presenting specific numerical simulation results.

For the purpose of illustration, Fig. 14 presents screenshots of the implemented and connected simulation models. The simulation environment can be used to evaluate the overall system behavior as well as the effects of specific improvement measures on different scales.

4.2 Product and process scale

Product agents store information about product characteristics determined by process models. This allows evaluating the effects of processes on product characteristics as well as the influences of existing product characteristics and process tolerances on subsequent characteristics. An example from the battery electrode production illustrates the capabilities of the simulation approach on product and process scale: Electrodes for battery cells are produced in batches along a process chain consisting of several processes starting with

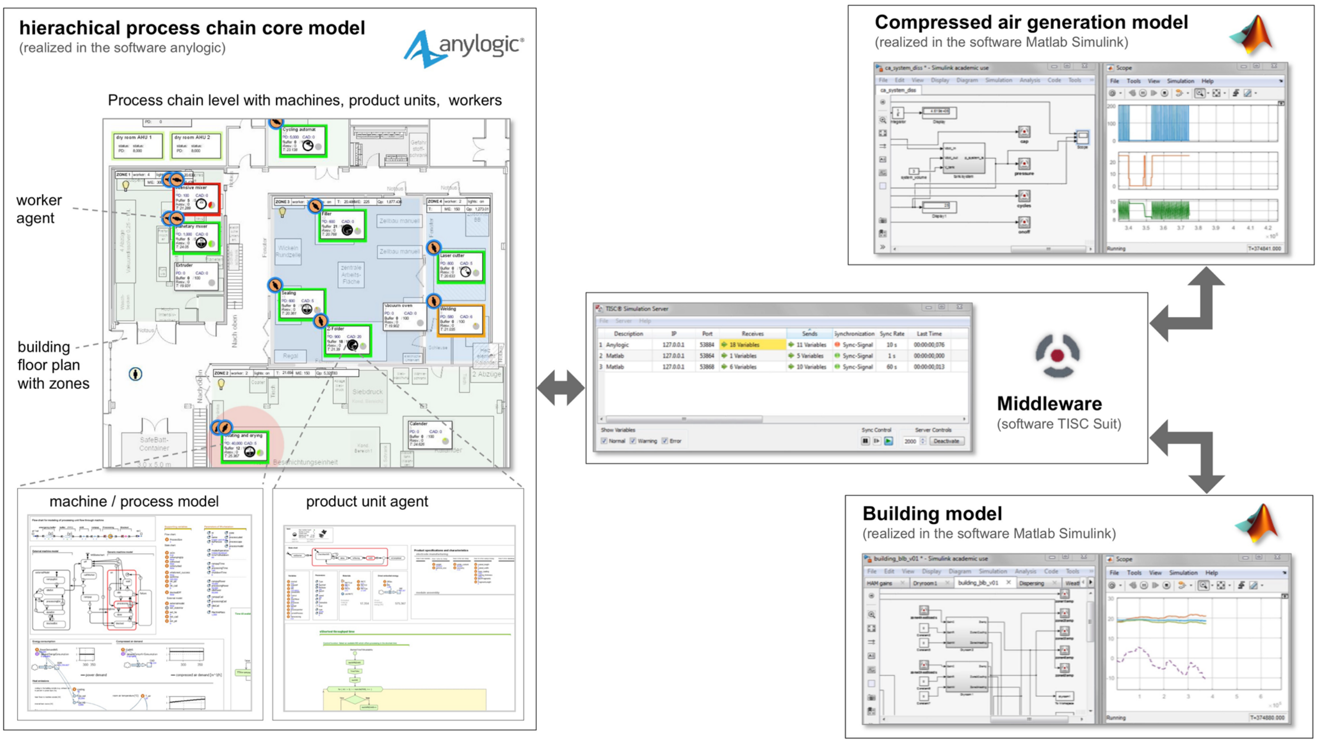


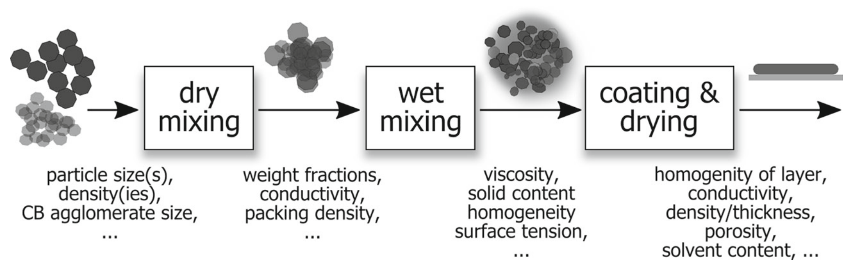
Fig. 14 Screenshot of process chain model with model instances of machines, processing units, and workers. Building zones are defined based on building ground plan and entities as well as heat emissions are assigned accordingly

dry and wet mixing of raw materials, coating of the resulting slurry onto a current collector foil, and drying of the wet electrode foil. All these processes influence the resulting product characteristics depending on the specific process configuration, formulations and parameters [61, 62]. For example, the mixing processes determine the quality of the produced slurry as well as important properties of this intermediate product, such as the viscosity of the slurry which subsequently effects the coating process and the resulting coating layer of the electrode foil [63, 64]. Thus, not only intermediate product properties are modified by process variations, but also substantial product properties such as density, porosity, and electrical resistance of the electrodes after coating and drying. Figure 15 shows the first processes of electrode production with relevant characteristics of intermediate products.

This following presentation of the simulation functionality observes only the modification of dry and wet mixing (dispersing) processes. The goal is to explain how the simulation can be used to evaluate the effects of different process configurations on the viscosity of the created slurry as well as on the characteristics of the produced electrode and the production system performance. For this purpose, four different process configurations for the slurry production have been considered, whereas the coating and drying processes as well as their parameters remain constant.

In the first reference scenario (REF), active materials (AM), binder (B), and carbon black (CB) are first combined in a dry mixing process before NMP solvent is added in a dispersing process. In the second scenario (KN), NMP solvent is gradually added in multiple dispersing steps. In the third scenario (BM), instead of metering B and NMP

Fig. 15 Processes of electrode manufacturing and related characteristics of materials and intermediate products



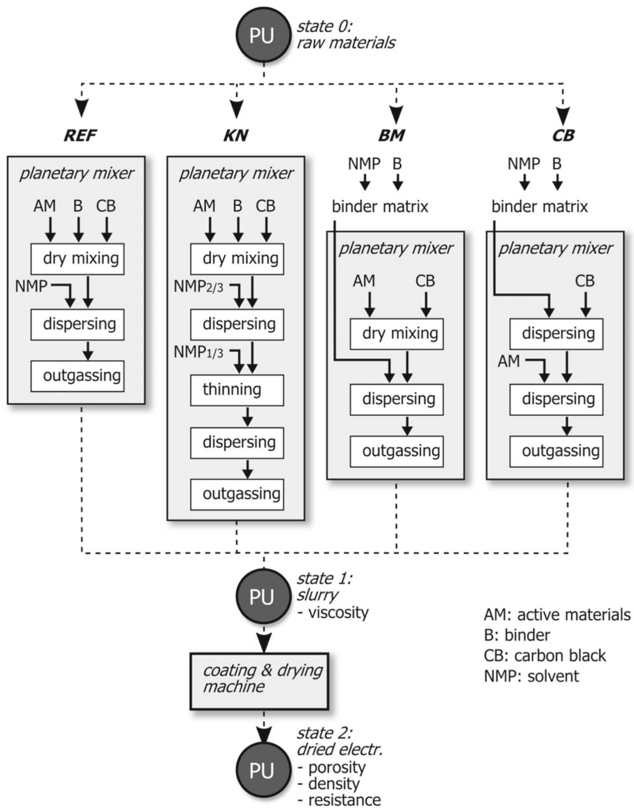


Fig. 16 Illustration of four scenarios for slurry production: reference, knead (KN), BM, CB

separately, a binder matrix is added in the dispersing step. In the last scenario (CB), forgoing the dry mixing step, CB is dispersed in a binder matrix and AM is dispersed herein subsequently. Figure 16 illustrates the process routes and configuration for the four scenarios.

Each scenario results in different processing times for the slurry production and power demand profiles of the used planetary mixer (since the total energy input into the slurry is kept constant in this example, only the power demand profile but not the energy demand is changed). The simulation allows evaluating these effects on resulting product characteristics, lead times for electrode production as well as the equipment utilization and power demand profiles of the entire factory .

Table 2 presents exemplary obtainable results for the defined scenarios.

The lead-time (LT) represents the overall time required for the production of one electrode batch from the first mixing step to the coated electrode foil. The time is only effected by the different processing times of the dry and wet mixing steps. The process time for coating and drying as well as time shares for handling and setup are kept constant. In general, the required process times influence the utilization of the production system and determine the possible quantity of electrode batches, which can be produced during an observed time period (e.g., a shift or a week). The resulting product characteristics are determined based on empirical process models. Measurements from experiments have been used to derive regression functions, which provide resulting characteristics based on process parameters. These models also contain information about the process tolerances in terms of the related standard deviation for the resulting characteristics. This allows assigning values for product characteristics for each product unit (batch) also based on probability functions during the simulation. The values show, that the process configuration from scenario KN results in a shorter lead-time, a lower viscosity of the slurry, a higher density, and a low electrical resistance of the electrode. And although these numerical values are only valid for specific assumptions, they show which types of simulation results can be acquired and how they enable a combined evaluation of different process configurations on product quality and production cost (e.g., as in [60]). The specific effects of process parameters on the machines operation as well as on the resulting utilization and power demand of the entire production system can be analyzed on process chain and factory scale.

4.3 Process chain and factory scale

The simulation allows determining the overall performance of the facility measured by different aggregated KPI. The flow and processing of product units determines the utilization and power demand profiles of the installed equipment. This also enables detecting bottlenecks and lead times of different jobs. Moreover, it is possible to observe the effects of heat emissions from machines as well as of

Table 2 Results for scenarios (S) of electrode production: Lead time (LT) per batch, viscosity (visc.), density (dens.), el. resistance (resist.), each with standard deviation (stdw)

S	LT [min]	visc.; stdw. [Pa*s]	dens.; stdw. [g/cm^3]	resist.; stdw. [Ohm]
REF	274	2.86; 0.10	2.29; 0.069	2.38; 0.09
KN	250	1.28; 0.05	2.48; 0.074	1.71; 0.06
BM	275	2.95; 0.10	2.28; 0.069	2.40; 0.09
CB	284	5.37; 0.20	2.17; 0.065	2.79; 0.10

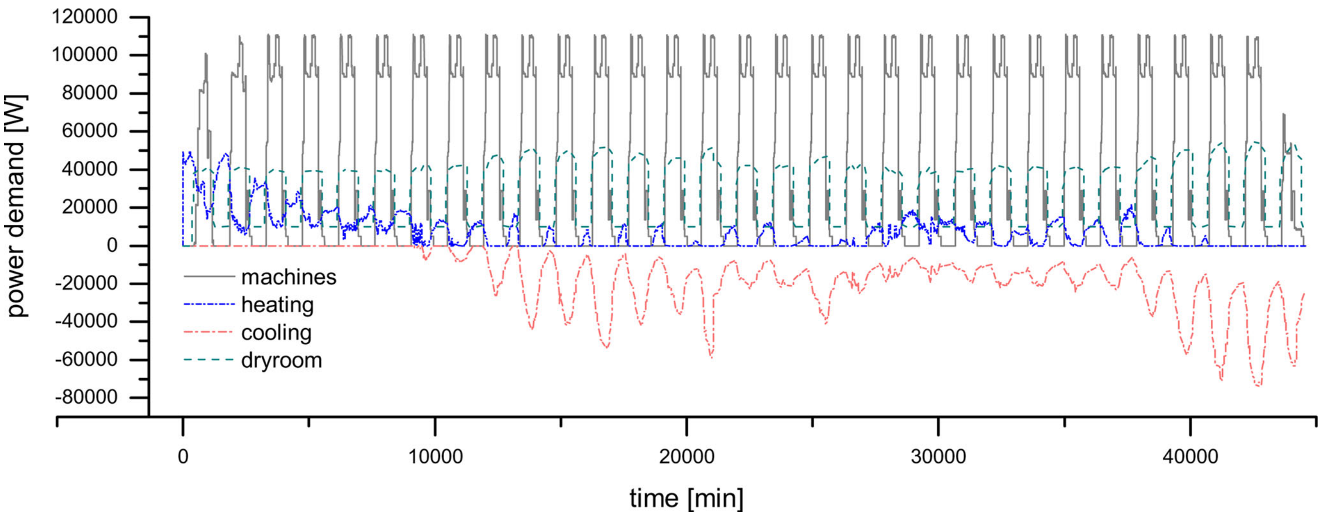


Fig. 17 Exemplary plots of power demands of equipment for one scenario during one month of production (including ramp-up and ramp-down). From top to bottom: power demand (watts) of machines, heating and cooling (cooling is shown as negative heating power demand), dry room (ventilation, dehumidification)

weather conditions on the building ambient conditions and required HVAC operation.

Different planning and evaluation tasks can be addressed by specific simulation runs, in which the effects of specific measures on the production system are determined. Examples of evaluation tasks are as follows: evaluation of different drying temperatures and drying times (to improve the drying process), additional machines (to address bottlenecks), different solvents within the slurry (which do or do not require air treatment systems), or different weather conditions.

As one exemplary result, the power demands for all equipment classes can be aggregated to load profiles and total energy demands. This enables identifying the most relevant equipment regarding energy costs or utilization. Figure 17 shows exemplary plots for the electrical power demands of machines, the dry room ventilation, and inlet air-cooling as well as the building heating and cooling for the period of 1 month.

While the machine load profile shows a rather similar pattern for each day, the heating and cooling demands depend on the weather condition. A higher outside temperature leads to an increase in energy demand for building cooling (negative values indicate cooling demand). The power demand of the dry room operation also shows a slightly increasing power demand for periods with warmer outside temperature.

The results further allow identifying the energy demands of each used production equipment during the observed time period and for the defined production scenario. Figure 18 shows the energy demands per system which reveals that—for the given scenario—the most energy is required for maintaining the building ambient conditions and for the coating and drying processes.

4.4 Summary of simulation study

Overall, the exemplary study shows the principles of multiscale simulation and obtainable results. And although the actual numerical results must be interpreted in the light of the made assumptions and the exemplary model character, they demonstrate how a multiscale approach can support planning and improvement of complex production systems.

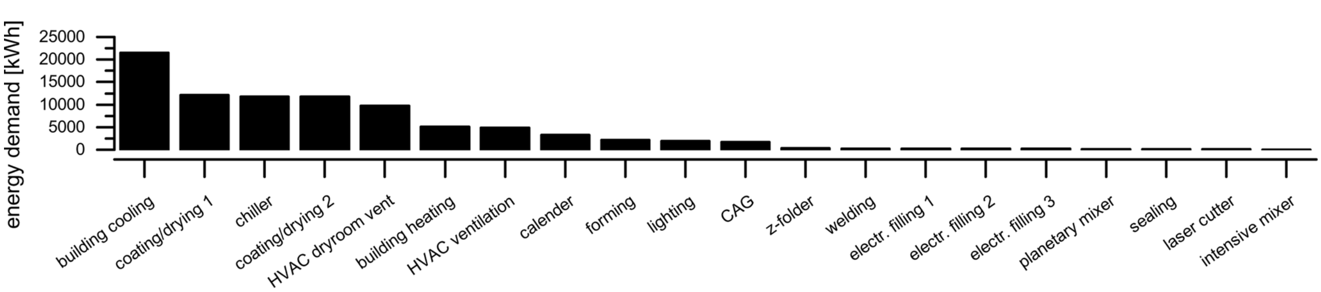


Fig. 18 Exemplary energy demand of equipment during 1 month of production for a specific planning scenario

5 Conclusion and outlook

The proposed concept for multiscale simulations supports the development of specific simulation applications for entire production systems. Although the idea of holistic production system simulations is not new, the concept is unique due to the combined consideration of economic, environmental, and technological aspects on multiple scales from single product units to the surrounding building. An important innovative feature is the agent-based process chain model concept. It enables the detailed evaluation of the relations between processes and product characteristics along the process chain and the required operation of machines as well as the aggregated energy and material demands, the system utilization, time shares and heat emissions. The coupling of specific detailed models for processes, machines, technical building services and the building structure enables a comprehensive analysis of the production system behavior. Such modular simulation can be used for different planning tasks and enable a close collaboration of involved disciplines.

However, there are some challenges of large multiscale simulations. The development of various models is time-consuming and requires interdisciplinary expert knowledge. Especially detailed numerical process models are very difficult to achieve since often many experiments are needed to derive knowledge about the process behavior. Thus, it is important to elaborate application procedures and organizational measures for the use of such simulations in production organizations and the reuse of existing sub-models. Furthermore, coupling of simulation models is a challenging tasks, especially since many established software tools do not provide the necessary interfaces for information exchange and co-simulation. Consequently, it is important to enhance established commercial software tools to ensure a time efficient execution of co-simulations based on models created in different software.

In the future, besides the evaluation of production systems, holistic multiscale production simulation could also be used for operational production planning and control by providing simulation results in real time to predict and control the production system operation. If required computational resources and interfaces to control tools are available, this is a promising approach since simulation could incorporate the evaluation of different scenarios, stochastic effects and algorithms for intelligent decision making into production control.

Funding information The data collection and model development for the exemplary case study was greatly supported by many researchers from the Battey LabFactory Braunschweig (BLB) in the context of the research project “DaLion” funded by the German Federal Ministry for Economic Affairs and Energy (BMWi; 03ET6089). The specific data for the electrode production are results of the research project “iFaaB” funded by the German Federal Ministry of Education and Research (BMBF; 02PJ2511).

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