

Sustainable Production, Life Cycle Engineering and Management
Series Editors: Christoph Herrmann, Sami Kara

Malte Schönemann

Multiscale Simulation Approach for Battery Production Systems

 Springer

Sustainable Production, Life Cycle Engineering and Management

Series editors

Christoph Herrmann, Braunschweig, Germany
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Modern production enables a high standard of living worldwide through products and services. Global responsibility requires a comprehensive integration of sustainable development fostered by new paradigms, innovative technologies, methods and tools as well as business models. Minimizing material and energy usage, adapting material and energy flows to better fit natural process capacities, and changing consumption behaviour are important aspects of future production. A life cycle perspective and an integrated economic, ecological and social evaluation are essential requirements in management and engineering. This series will focus on the issues and latest developments towards sustainability in production based on life cycle thinking.

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Multiscale Simulation Approach for Battery Production Systems

 Springer

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Foreword

Manufacturing companies play an important role in the transition to a global sustainable development. They create products by using resources such as materials and energy, which in return cause various emissions to the environment, and directly or indirectly affect the well-being of people. Consequently, the goal must be to improve the production operation to reduce costs and environmental impacts while creating products with a desired quality. This is no easy task since prevalent cause–effect relationships in production systems bear the risk of problem shifting. In particular, this is relevant for the production of complex products which require various processes, diverse equipment, and specific factories. Well-intended measures and the utilization of innovative technologies may lead not only to local improvements, but also to undesired effects in other sectors or equipment of a production system causing higher overall costs and environmental impacts. In order to avoid problem shifting, production engineers and product developers need methods and tools for an integrated decision support and to foster the collaboration of these disciplines to gain an interdisciplinary system understanding. In this regard, simulation is a powerful method which enables to examine the dynamic behavior of complex systems. However, due to the high effort related to the creation and employment of sophisticated simulation models, the application of simulation in industry is so far limited.

With this published work, Schönemann has strongly contributed to the application of simulation for planning and improvement of production systems and products. He developed a multiscale simulation approach with an exemplary application for the case of large scale battery systems production which considers the relevant characteristics and elements of production systems needed for the integrated evaluation of economic, environmental, and technological goals. His approach is based on coupled simulation models allowing the utilization of best-suited modeling approaches and tools to represent specific production system elements in detail. As an example of a detailed model, he suggests an agent-based process chain simulation in order to consider the characteristics and production requirements of individual product units. This is novel in contrast to established

process chain simulation approaches. In addition, he defined interfaces between different model types to enable the use of existing models and to increase the re-usability of models, which reduces the effort for model creation and fosters the collaboration of different disciplines and experts. Although being specifically developed for battery production systems, the approach stands on a generalized framework which allows an easy adaptation also to other industries.

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Malte Schönemann

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Acronyms

AHU	Air handling unit
AB	Agent based
BCVTB	Building control virtual test bed
BMS	Battery management system
CB	Carbon black
DE	Discrete event
DEM	Discrete element method
DS	Dynamic systems
FEM	Finite element method
GWP	Global warming potential
HLA	High level architecture
HVAC	Heating, ventilation and air conditioning
LCA	Life cycle assessment
LCI	Life cycle inventory
Li	Lithium
LIB	Lithium-ion battery
LMO	Lithium-Mangan-Oxid
MTTF	Mean time to failure
MTTR	Mean time to repair
NMP	N-methylpyrrolidone
OCV	Open circuit voltage
PHEV	Plugin hybrid electric vehicle
PMI	Process machine interaction
PVDF	Polyvinylidene fluoride
SD	System dynamics
SEI	Solid electrolyte interphase
SOC	State of charge
TBS	Technical building services
TRY	Test reference year
VSM	Value stream mapping

Symbols

A_{mn}	Surface area of machine with number mn
A_d	Window surface area
A_w	Wall surface area
α_{mn}	Convective heat transfer coefficient of machine with number mn
acr	Air change rate
BC_{mn}	Buffer capacity of machine with number mn
J_{jn}	Job with job number as index ($jn = 1, \dots, JN$)
C_{energy}	Total energy costs
$C_{machining}$	Total costs of machine operation
$C_{materials}$	Total material costs
c_{mn}	Heat capacity of machine with number mn
C_{total}	Total production costs
CAD_{MACH}	Compressed air demand of all machines
$CAD_{MACH_{mn}}$	Compressed air demand of machine with number mn
CAD_{mn_c}	Compressed air demand of component c or machine with number mn
CO_2^{eq}	Equivalent carbon dioxide
DED_{pun}	Direct energy demand of processing unit with the number pun
EI_{energy}	Environmental impact of energy generation
$EI_{materials}$	Environmental impact of materials
ε_{mn}	Emissivity factor of machine with number mn
g	Energy transmittance
I_{max}	Maximum radiation
$MACH_{mn}$	Machines with machine number as index ($mn = 1, \dots, MN$)
m_{air}	Mass of air
m_{mn}	Mass of machine with number mn
$\dot{M}E_{WO_{wn}}$	Moisture emissions of worker with number wn
$PCHAR_{ptn}$	Product characteristics
PD_{MACH}	Power demand of all machines
$PD_{MACH_{mn}}$	Power demand of machines with number mn

$PD_{mn,c}$	Power demand of component c ($c = 1, \dots, C$) of machine with number mn
PD_{CAG}	Power demand of compressed air generation
PD_{HVAC}	Power demand of HVAC systems
PD_{LIGHTS}	Power demand of lighting
PD_{TBS}	Power demand of entire TBS
PD_{TOTAL}	Total power demand of entire process chain
PT_{ptn}	Product type with product type number ptn as index ($ptn = 1, \dots, PTN$)
PU_{pun}^{ptn}	Processing unit with processing unit number pun as index ($pun = 1, \dots, PUN$) and associated product type ptn
$\dot{Q}_{HS_{mn}}$	Heat source within machine with number mn
\dot{Q}_{WO}	Heat emissions from workers
$\dot{Q}_{WO_{wn}}$	Heat emissions from worker with number wn
\dot{Q}_{LIGHTS}	Heat emissions from lighting
\dot{Q}_{MACH}	Heat emissions from all machines
$\dot{Q}_{MACH_{mn}}$	Heat emissions from machine with number mn
$\dot{Q}_{mn,c}$	Heat emissions from component c of machine with number mn
\dot{Q}_{TOTAL}	Total heat emissions to the building
σ	Stefan-Boltzmann constant
$T_{air,z}$	Air temperature of building zone z
T_{mn}	Surface temperature of machine with number mn
U_w	Heat transfer coefficient of a wall

Chapter 1

Introduction

Battery systems for energy storage are among the most relevant technologies of the 21st century. They – in particular modern lithium-ion batteries (LIB) – are enablers for the market success of electric vehicles (EV) as well as for stationary energy storage solutions for balancing fluctuations in electricity grids resulting from the integration of renewable energy sources with volatile supply¹. Both EV and stationary storage solutions are important because they foster the transition from the usage of fossil energy carriers towards cleaner renewable energy sources. Furthermore, EV cause less local air pollution and noise emissions compared to conventional combustion engine vehicles resulting in better air quality especially in urban areas. Unfortunately, to this day, various technological and economic challenges impede a broad application of batteries for EV as well as for large scale energy storage and load leveling in electricity grids.

In 2010, the German government has set the goal of 1 million registered EV in Germany by 2020 (NPE 2010). This goal is motivated by the commitment to reduce carbon dioxide emissions of the transport sector as well as to establish Germany as a lead provider and market for electric mobility technologies. Until today, however, this goal seems far from reachable, even if hybrid electric vehicles (HEV) are included in the electric vehicle stock. Figure 1.1 shows provocatively the development of the stock of EV in Germany from 2006 until 2016 in reference to the goal of one million vehicles (without HEV). The plot is hardly visible in the figure since only 25,502 EV were registered in 2016 (January). Consequently, a strong growth in new registrations

¹In addition to EV and stationary storage, batteries are essential components for portable and mobile consumer electronics. The predicted market shares (based on revenue breakdown) of these three segments of LIB application in 2020 are 37.6% for grid and energy storage, 30% for automotive applications and 23.9% for consumer electronics. Other industrial applications account only for 8.5% (Frost and Sullivan 2014).

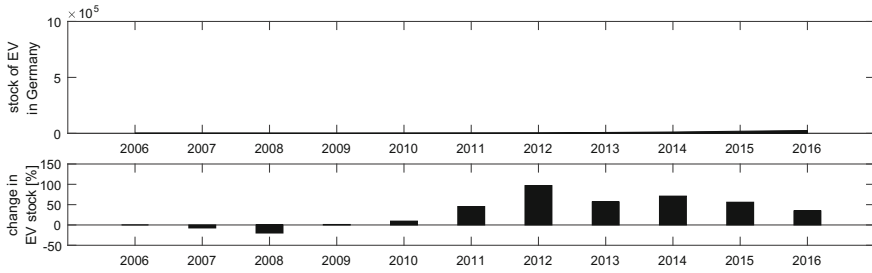


Fig. 1.1 *Top* Development of the stock of EV in Germany from 2006 to 2016 in reference with the goal of 1 million registered EV in Germany by 2020 (without HEV). *Bottom* Annual change in EV stock in percent (KBA 2015, 2016)

is required to approach the set goal. However, the figure further presents the annual development of the vehicle stock and it reveals that there is no consistent increase in new vehicle registrations.

The barriers of a successful and broad commercialization of EV are high vehicle costs, short driving ranges, and long charging times (Braess and Seiffert 2013). In this regard, battery systems are among the most important vehicle components (Hettesheimer et al. 2013). The production costs of battery systems² can account for up to 40% of the total production costs of a vehicle (Acatech 2010). This leads to much higher sales prices of EV compared to conventional vehicles. This aspect becomes even more relevant considering the relatively short life time of battery cells. Their capacity decreases with age and used cycles and consequently the battery system will likely have to be replaced during the life time of a vehicle. Furthermore, the driving range of an EV depends on the energy density³ of the battery system. Since the size of a battery system is limited by the available space within a vehicle structure and weight restrictions, the achievable capacity only enables a relatively short driving range. In addition to these technological shortcomings, the production of battery systems entails high environmental impacts due to the used materials and required production processes. For example, Volkswagen states that the battery system can contribute to up to 45% of the production related CO₂ emissions of a vehicle, whereas 36% can be allocated to the production of battery cells (Volkswagen AG 2012). Similar, Hawkins et al. mention the share of 35–41% for the battery production on the global warming potential (GWP) of the vehicle production phase (Hawkins et al. 2013). Overall, these numbers underline that battery systems are very important components of EV. The market success of EV depends on the improvement of the performance of battery systems and cells (i.e. energy and power density, cycling stability,⁴ charging

²According to Nykvist and Nilsson (2015), the production costs of battery cells for automotive OEM are currently around US\$ 300–400 per kWh; further decline is expected.

³Gravimetric (Wh/kg) and volumetric (Wh/l) energy density. Modern LIB have energy densities around 230 Wh/kg (Nishi 2014).

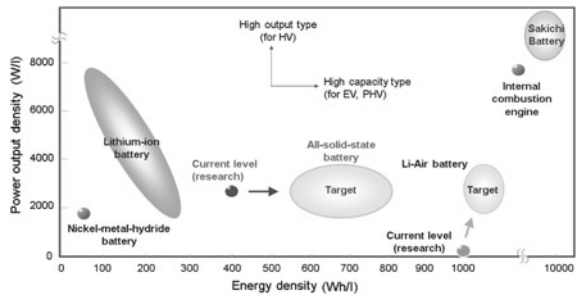
⁴The cycling stability is characterized by the number of charging and discharging cycles until the battery capacity degrades to 80% of the initial capacity (Dinger et al. 2010).

times, etc.) and a reduction of their production costs. Decreasing production costs will also foster the usage of batteries for stationary energy storage applications. This could in return increase the production volume supporting economies of scale. Furthermore, from an environmental perspective, it is important to reduce the negative environmental impacts related to cell production. If batteries harm the environment, they foil the intention behind EV and renewable energy sources which is to unburden the environment of the impacts from transportation and energy generation.

The German engineering association VDMA⁵ published a road map for battery production technology and named four grand challenges (VDMA 2014). The first challenge is the scale up of processes from laboratory scales to series production with high volumes. It is necessary to achieve short throughput times although facing uncertain demands. Second, process stability has to be improved to increase the output by reducing the scrap rate. The third challenge is sustainability in battery production addressing the used materials in products and processes as well as energy and resource efficiency. The last challenge is the reduction of production costs while improving the product quality.

In addition, another challenge is the expected evolution in battery technology. Today, LIB are the most established batteries of which producers have the most experience and know-how regarding material combinations and large scale mass production. However, new material systems such as lithium-air and new battery types such as all solid state batteries are currently in development. Although these so-called next-generation batteries are still only available in laboratory scale and have not proven to be advantageous for large scale production, they will be relevant in the future. Toyota already presented a road map towards lithium-air batteries (Yada et al. 2015; Mizuno et al. 2014). Figure 1.2 shows a ragone plot of the energy and power densities of different battery types. Thus, it is expected that the required production technology and production steps will evolve together with new battery systems. Consequently, these future developments have to be considered in present improvements of battery production and in the evaluation of investments in production technology. Finding solutions to the described challenges is of great importance to producers of batteries and related production equipment.

Fig. 1.2 Ragone plots of established and next-generation battery systems (Mizuno et al. 2014)



⁵Verband Deutscher Maschinen- und Anlagenbau e.V.

Today, the majority of battery cells is produced in Asia.⁶ However, Tesla⁷ is currently building a gigafactory for battery cells in the USA with an annual production capacity of 35 GWh. This capacity would be higher than the entire global production capacity for battery cells in 2013. Tesla's goal is to achieve a reduction in production costs of 40–45%. Companies from other countries – including Germany – produce only a small number of battery cells per year. In this situation, the challenges and drivers for improvements may be different for each battery producer. While the established market participants aim at improved battery performance and reduced production costs by optimizing their production systems and product designs, aspiring companies have to establish a competitive battery production facing high risks from uncertain demands and low but potentially increasing production volumes. Moreover, established producers have to find ways for integrating new battery technologies into existing production systems while new production facilities may account for future battery technologies already from the beginning. In general, it is important to tackle the described challenges of battery production by developing innovative production technologies and strategies along with product designs which enable a flexible scale up as well as an economic and environmental friendly production. Figure 1.3 summarizes the challenges and drivers for the improvement of battery production as well as the relevant goals.

The goals are strongly interlinked since the battery performance depends on product specifications, materials, and process characteristics (e.g. quality rate or process parameters), all of which also effect the production costs and environmental impacts related to production processes. For example, the specified power and energy of a battery have strong influence on production costs (Gallagher and Nelson 2014). As another example, the substitution of battery materials (e.g. active materials or solvents) may require different process parameters (e.g. mixing intensity or drying time) or equipment which can effect the energy demands of machines, the utilization of resources, and the output of product units per production time. That means that improvement measures regarding one goal may result in problem shifting causing negative effects regarding other goals. Consequently, it is important to find improvement measures which avoid problem shifting between different production system elements and the defined goals. However, the various and often dynamic relations

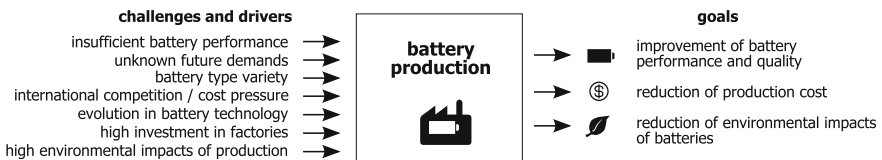


Fig. 1.3 Challenges, drivers, and goals of battery production

⁶More specifically, the countries with the highest production volume are Japan (by far with 19,200 MWh; Panasonic and Samsung), Korea (LG) and China (BYD). This order is based on the expected market shares in 2017 (Roland Berger Strategy Consultants 2015).

⁷Tesla Motors, Inc.

within a battery production system (e.g. between machines, processes, materials, building infrastructure, material and information flows, etc.) result in complex system characteristics which are difficult to be completely understood intuitively by engineers. Thus, there is a need for methods and tools supporting an interdisciplinary system understanding which fosters innovations and an integrated evaluation of improvement measures regarding all goals. Such methods and tools must address the following fields of action:

- Identification and reduction of inefficiencies and non-value adding activities within the production system
- Identification of energetic hot spots and reduction of energy demands of processes and auxiliary equipment
- Identification and analysis of influences from production processes on product characteristics along the process chain, and vice versa
- Derivation and evaluation of product specifications and production strategies aiming at defined improvement targets (such as “high performance battery”, “environmental friendly battery”, or “budget battery”)

However, no methods and tools for the integrated evaluation of measures are already established or available for application. So far, only specific approaches have been developed addressing either the technological, economic, or environmental evaluation of batteries, battery components, or production systems. The technical performance of batteries is often analyzed with simulations on electrode, cell, module, or system level. Physical models are used to determine performance indicators for specific cells or batteries. Economic aspects and in particular the production costs of batteries are addressed in various studies and cost models. The environmental impacts of batteries are analyzed in several life cycle assessment (LCA) studies. However, the published LCA studies from the last few years have shown different results for the energy consumption in cell production (Ellingsen et al. 2014). Studies of the energy demand strongly rely on rough estimations and assumptions. For example, some studies assume that factories operate at full capacity – which is often not the case – or refer to a lab-scale production system. This affects the results since energy demands depend on the used equipment and process parameters and vary over time along with the production output. Also, often specialized building equipment such as dry rooms are not included in the studies at all or not considering the actual output of products. Hence, it has not been possible to allocate the energy demands of peripheral production equipment on single product units (Dunn et al. 2014). Furthermore, static methods such as LCA or cost calculations have shortcomings regarding the consideration of dynamic effects. Since the challenges of battery production are especially caused by the dynamic behavior and interactions of different production system elements, static methods seem not suitable for an integrated evaluation. Instead, dynamics in production systems can be replicated and analyzed by simulation methods. In production engineering, discrete event simulations are in use for the evaluation of process chain performance and logistic related planning tasks but are not capable of simulating physical production process in detail. Detailed physical models, however, are usable for the simulation of

continuous processes but not well suited for modeling of discrete activities on production system level. Other disciplines (e.g. material science or civil engineering) use hybrid or so-called multiscale simulation approaches to analyze and solve multi-domain engineering problems. This concept was already applied to the simulation of production systems but mostly with a focus on energy management in factories without considering a detailed product perspective. In conclusion, no model based evaluation method exists for production systems which allows considering dynamic interactions between product specification, production processes, the production system operation, and factory infrastructure as well as between technological, economic and environmental objectives. However, according to Forrester (1994) – the initiator of the system dynamics approach – modeling and computer simulation help to gain insight into the dynamic behavior of complex systems. Modeling is part of an iterative learning process which results in an improved system understanding of the involved stakeholders (Sterman 2000).

What is strongly required for the improvement of battery production is a new modeling method for supporting the evaluation of improvement measures regarding technological, economic, and environmental objectives as well as for generating an interdisciplinary system understanding of battery production, as illustrated in Fig. 1.4.

The goal of this work is to develop such multiscale simulation method which contributes to the improvement of battery systems for EV and stationary energy storage solutions as well as their production systems. Such method must address different planning perspectives such as strategic, tactical and operational planning (different time scales) and consider all production system elements such as product units, processes, machines, technical building services (TBS) and the building (different spatial scales) and their dynamic interactions. For example, products are transformed by processes in machines, machines are organized in process chains, the operation of TBS depends on the activities within the process chain and the environmental conditions inside and outside of the factory building. For these reasons, there is a need for a hybrid multiscale simulation approach which allows to accurately imitate the production activity and to determine performance indicators of production systems and produced batteries or components for a later evaluation.

Beside addressing the described challenges, this desired planning method must enable the evaluation of future battery technologies. This creates the demand for a planning and evaluation method which is usable also for next-generation batteries which are not specified today.

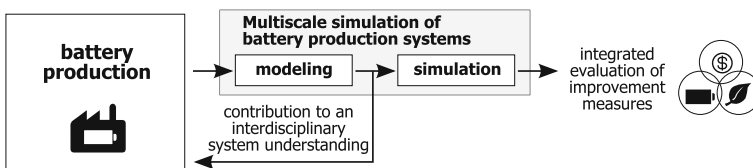


Fig. 1.4 Motivation for a multiscale simulation of battery production

The developed concept shall be transformed into a functional model which serves the evaluation of the concept and the intended evaluation tasks. This book is structured into seven chapters of which the content is shortly described in the next paragraphs.

- Chapter 2** presents the relevant background information needed to create a multiscale simulation of battery production systems. This includes knowledge about the structure of battery systems, production systems and management, as well as the simulation methodology with current trends, strategies, and approaches for the development of simulation applications for production systems. The chapter concludes with a summary of relevant aspects of battery production which have to be considered in a simulation concept.
- Chapter 3** presents the state of research regarding multiscale simulation approaches for production systems. The chapter evaluates existing research contributions and derives research demands towards a multiscale simulation of battery production systems. It reveals that although different simulation approaches and methods as well as various specialized simulation models (e.g. for machines, HVAC systems, buildings) exist, no approach was found providing the required functionality to combine simulation results from product and process scale up to the building.
- Chapter 4** presents the development of the multiscale simulation concept for battery production systems. In particular, it describes the objectives and requirements for the simulation concept, a framework as a pattern for model interactions, the content and logic of models for required production system elements and the coupling of different models. The core of the concept is a process chain model which allows to model products and machines as agents sharing information about their characteristics and states. Furthermore, an application procedure is described which supports developers of such multiscale simulation models in selecting and modeling production system elements, and in using the resulting simulation environment.
- Chapter 5** presents the implementation of a multiscale core model which acts as a coordinator for detailed models. This model enables the evaluation of the functionality of the proposed simulation concept. It provides all models, parameters and variables which are required to demonstrate the simulation of any kind of production system configuration for battery production. Moreover, for the purpose of demonstration and for the verification of the model coupling, a detailed model of a compressed air generation system was developed and connected to the core model via a middleware software. Furthermore, the section explains the verification of the core model with its integrated sub-models, the detailed compressed air model and an analysis of the effects of the model coupling on simulation results.
- Chapter 6** demonstrates the application of the simulation concept by creating two exemplary multiscale simulations for cell production and system assem-

bly. The first case study investigated the cell production at the Battery LabFactory Braunschweig which is a laboratory scale production facility. The second case is the assembly of different types of battery systems on one assembly system. Both case studies demonstrate the application of a multiscale simulation.

Chapter 7 summarizes the results of this work, presents a critical review of the concept, and gives recommendations for further research activities.

Figure 1.5 illustrates the structure of this book.

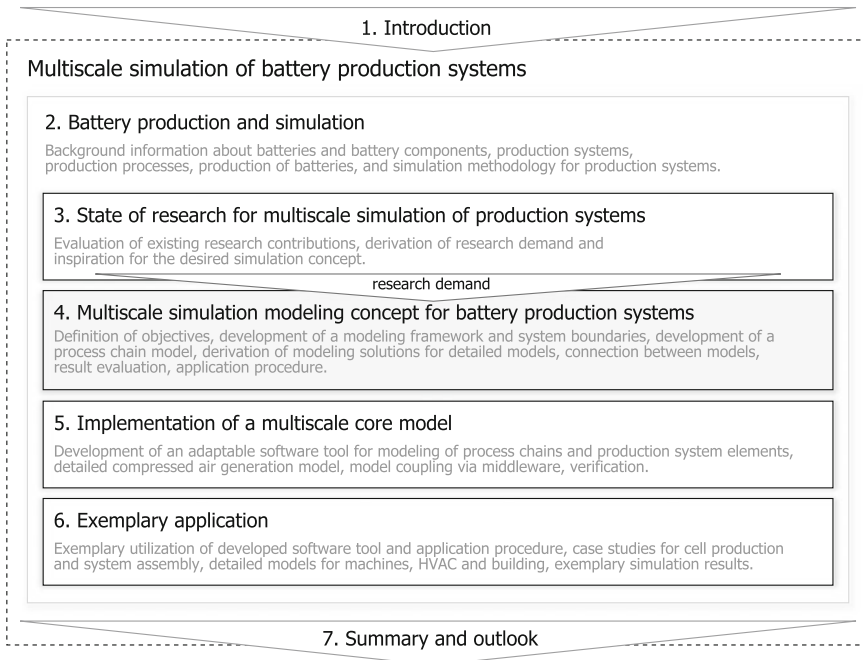


Fig. 1.5 Outline of the book

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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).

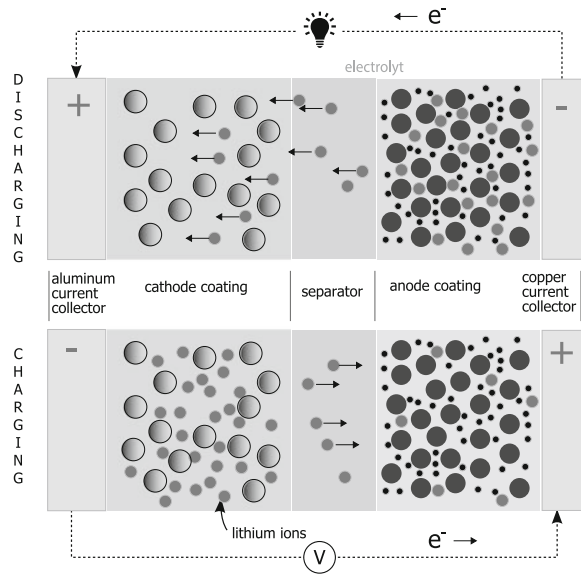
2.1.1 Batteries and Battery Components

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



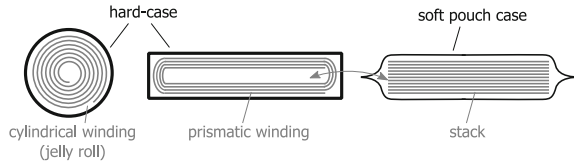
released electrons are conducted through an external circuit from the anode to the cathode. During charging, the direction of the movement of electrons and lithium ions is reversed by a connected power supply. Figure 2.1 illustrates these reactions and the structure of a LIB cell.

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.

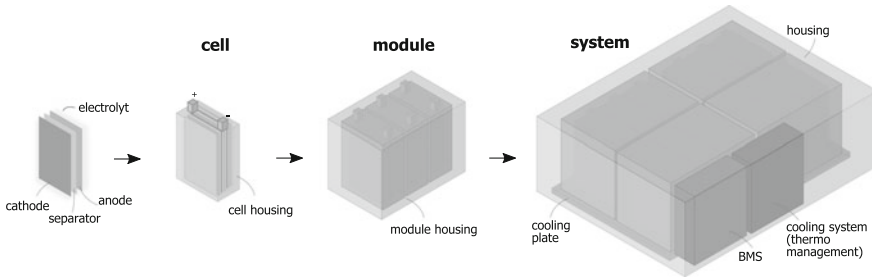


Fig. 2.3 Illustration of an exemplary battery system structure

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 casing. 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

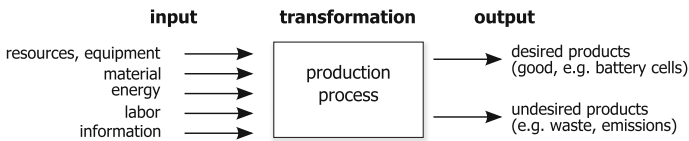


Fig. 2.4 Production as physical transformation process according to Dyckhoff and Spengler (2010) and Schenk et al. (2014)

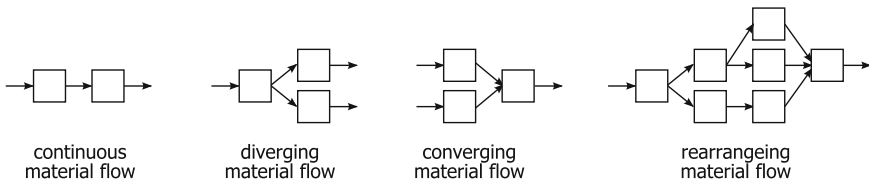


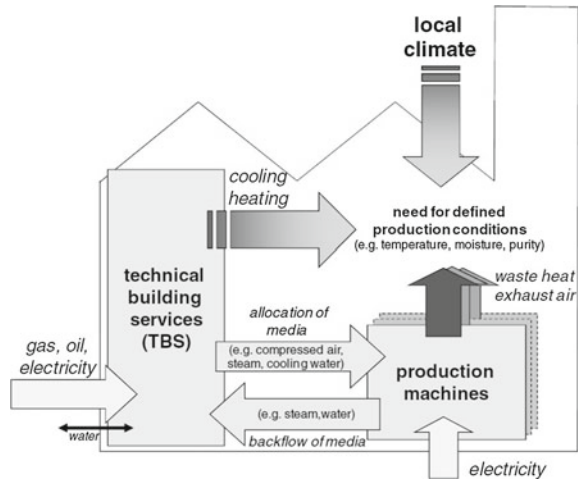
Fig. 2.5 Types of material flows according to Dyckhoff and Spengler (2010)

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)

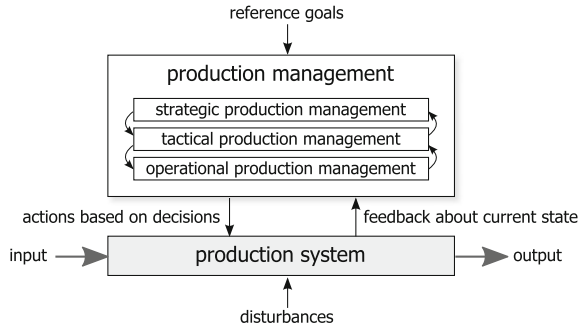


Verl et al. (2011) additionally including the supply chain or global production system as the highest level above the factory level. Schenk et al. (2014) present a hierarchy of sub-systems of a production system based on peripheral orders. Another kind of hierarchy is developed by Nylund and Andersson (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

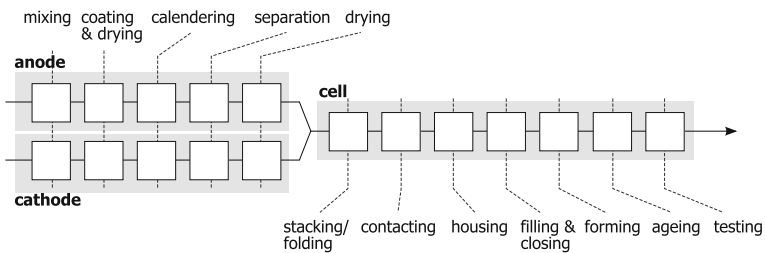


Fig. 2.8 Process chain of lithium-ion battery cells for stacking or folding cell assembly

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.

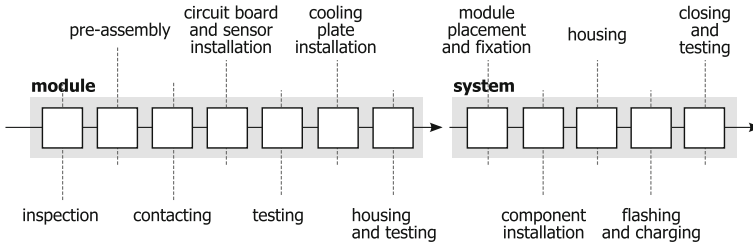


Fig. 2.9 Process chain of battery module and system assembly

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 cleanness in building zones since temperature, humidity, and cleanness 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

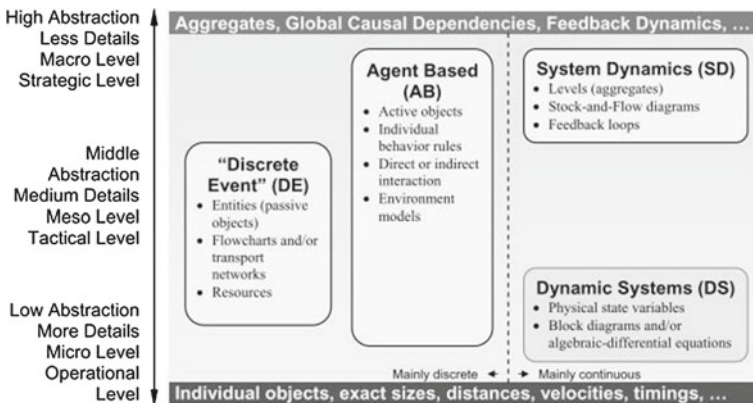


Fig. 2.10 Simulation approaches on abstraction level scale from Borshchev and Filippov (2004)

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

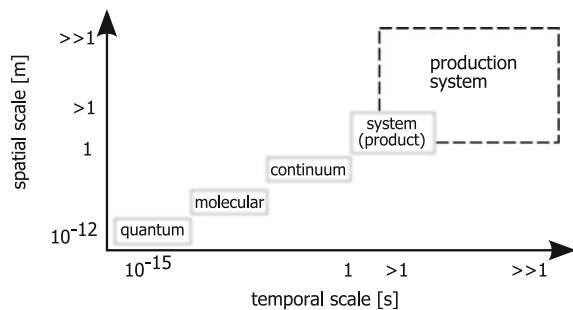
Many problems in science and engineering show multiscale solutions considering different spatial and temporal scales of individual systems or processes. The concept of multiscale modeling and simulation is established in various domains and disciplines such as biology (Boras et al. 2015), material science 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)



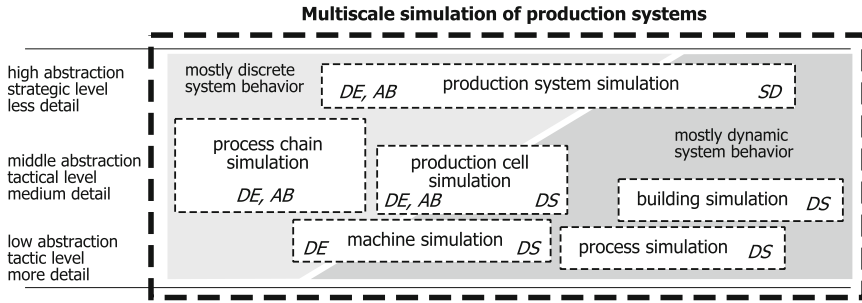


Fig. 2.12 Structure of simulation models for different scales considering suitable simulation approaches; figure inspired by Borshchev and Filippov (2004) and Landherr et al. (2013)

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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Chapter 3

State of Research for Multiscale Simulation of Production Systems

This chapter presents the state of research in areas related to multiscale simulation of production systems. There are various generic or specific simulation applications for production systems of which many were reviewed in order to provide an overview about existing approaches, underline the relevance of production system simulation, and to get inspiration for specific methodological solutions. This chapter explains the selection of reviewed approaches and the definition of evaluation criteria (Sect. 3.1) as well as the evaluation of the selected approaches (Sect. 3.2). The chapter concludes with an identified research demand (Sect. 3.3).

3.1 Selection of Approaches and Definition of Evaluation Criteria

There has been a wide range of applications of simulation for production systems and a multitude of simulation models and approaches. Consequently it is necessary to select relevant approaches (Sect. 3.1.1) and to define evaluation criteria according to the identified requirements for a detailed battery simulation (Sect. 3.1.2).

3.1.1 Selection of Approaches

In general, applicable simulations were considered which provide useful methods, techniques, and ideas for the multiscale simulation of discrete part production including different scales from the lowest process scale up to the building scale. In particular, three main research areas were examined which share goals and features similar to the intended multiscale simulation of battery production systems.

1. Simulations for the evaluation of production systems regarding economic and environmental objectives. In this context, simulations address the operational performance (e.g. output, lead time), material flows, and the related energy demands of the entire production equipment.
2. Simulations aiming at the analysis of product characteristics during production along a process chain and the acting effects of process parameters, machine configurations, and environmental conditions (technological objectives).
3. Simulations which combine different simulation models in order to improve the result quality regarding the desired objective.

Static applications such as linear programming models were not considered in this evaluation. These models are often used for planning and optimization tasks in the context of production systems but do not imitate the complex dynamic behavior of production systems over time. An example of such optimization model is published by Agha et al. (2010) in which an integrated approach is used to optimize the schedules of production operation and utility systems (boiler and fuel storage). Their concept addresses a multiscale analysis of production systems but the static optimization approach limits the application. Furthermore, contributions were not considered if they solely focus on simulation techniques in general aiming at optimized algorithms, IT infrastructures, and distributed computer systems (e.g. Sicklinger et al. 2014; Sweafford and Yoon 2013 or Viel and Minimes 2014).

3.1.2 Evaluation Criteria

The selected approaches have been evaluated regarding a set of criteria. These criteria were derived from the findings described in Sect. 2.3 and clustered into the groups scope, scales, as well as methodology and application. This subsection describes the criteria and the specification of criteria fulfillment.

Scope

The criteria related to the scope observe the relevance of a simulation application for battery production, the planning perspectives, and the addressed objectives.

Battery production relevance This criterion refers to the context of an approach.

The related question is, if an approach aims at simulating the production of batteries or if it is applicable or adaptable for the simulation of battery production systems. The criteria is not fulfilled if an approach is not related to or does not address the production of batteries or battery components. This criterion is completely fulfilled if the research is directly related or specifically designed to be applied to battery production. The criterion is partially fulfilled if an approach addresses discrete production and considers system elements or aspects relevant to battery production.

Multiple planning perspectives Production management can take operational, tactical, and strategic perspectives. The related question to this criterion is, if a simulation application supports planning tasks of all three perspectives or if it is limited to a specific perspective. In the best case, a simulation approach is able to support tasks from all planning perspectives. The criterion is not fulfilled if it is not possible to identify any addressed planning perspective.

Integrated objectives Product quality, production costs and environmental impacts during production are closely related. Consequently, it is desired to investigate the cause-effect relations between technological, economic, and environmental objectives in an integrated manner. The related question is, if a simulation application allows to consider all three objectives simultaneously or if only specific objectives are addressed, for example energy efficiency. The criteria is completely fulfilled if an approach addresses the integrated analysis of all three objectives. The criteria is not fulfilled, if no objective is clearly defined.

Production System Scales

The criteria related to the production system scales describe whether and in which detail a simulation application addresses single or multiple scales of a production system. For this evaluation, it has been differentiated between the scales process, product, machine, process chain, TBS and the building.

Process This criterion refers to the consideration of production processes in a simulation.¹ Processes can be described and modeled using different methods and levels of detail. The related question to this criterion is, if a simulation includes modeling of specific process characteristics and processing results in detail. This criterion is not fulfilled if process characteristics and the influences on product characteristics are not considered at all. It is fulfilled if physical models (e.g. using finite element methods (FEM) or discrete element methods (DEM)) are included for describing the detailed process characteristics. It is partially fulfilled if process characteristics are considered within other related models for machines or products. The degree of fulfillment depends on the modeled level of detail.

Product Processes transform an initial state of a product unit (or workpiece) into an output state which is characterized by the current product characteristics. This output product state can be the input of an adjacent process. This criterion refers to the consideration of product unit specific requirements for processing and created product characteristics within a simulation application. It is not fulfilled if product units and their characteristics are not considered at all. It is completely fulfilled if different product types, their specific requirements for processing and intermediate states of product units during production are integrated within a simulation and if the physical influences of processes and machines on product characteristics can be analyzed. It is partially fulfilled if a simulation considers product units

¹It was found that processes and machines are often treated and modeled synonymously. However, a machine is required to perform a process. A process is the activity which transforms the properties of a product to desired states or conditions.

as events, product specific parameters (e.g. processing times) for processes, or product units as black box models with a defined set of parameters.

Machines Machines consist of various components (e.g. mechanical parts, sensors, control) and have different states (e.g. idle, processing, failure) and operational characteristics (e.g. maximum values of process parameters, working area, capacity, availability, mean time to failure (MTTF), scrap rate). Furthermore, machines have energy and media demands (e.g. for compressed air, cooling liquid) which depend on the operational state. This criterion evaluates the consideration of machine characteristics in simulation approaches. The related question is, if an approach addresses the behavior of machines. This criterion is not fulfilled if machines are not specifically included in an approach and completely fulfilled, if detailed models of machines are used to represent structural and operational machine characteristics including machine component behavior.

Process chain Machines can be grouped to process chains according to their functionality or according to the desired process combinations for specific product types. Relevant plannings task related to process chains are for example the allocation and routing of products to machines, the scheduling of jobs, bottle neck and lead time reduction, and improvement of the systems utilization. This criterion refers to the consideration of the operation of multiple machines, material flow and product routing, schedules, and the overall production performance. It is not fulfilled if no coordinated process chain and product flow is included in an approach. It is completely fulfilled if the product flow and routing, buffers, and detailed scheduling are included and an evaluation of performance indicators as well as of impacts on TBS is possible.

Technical building services This criterion refers to the consideration of TBS and auxiliary equipment within a simulation application. TBS are related to machines (e.g. compressed air, air suction) or the building operation (e.g. HVAC, lighting, energy supply). The criterion is not fulfilled if TBS are not considered at all. It is completely fulfilled if all required services are included by in-depth physical models which represent the operation as well as the interactions with processes (e.g. demand/supply) and the building (e.g. heat emissions). The criteria is partially fulfilled if only few TBS are included which are only represented by simplified models.

Building This criterion specifies if a simulation supports the analysis of the building surrounding a production system. The simulation of buildings can be realized with different methods and tools and be carried out in different levels of detail. The related question is, if a simulation considers or includes the building ambient conditions. It is completely fulfilled if the building shell is a major part of a simulation and if detailed physical models are implemented to represent the building construction, weather influences, and internal loads. The criterion is not fulfilled if the building is not part of an approach. It is partially fulfilled if simplified models for building zones are used.

Methodology and Application

This group of criteria addresses the questions whether existing simulation applications use coupled simulation models, provide an integrated evaluation of results from different models, and are applicable to other production systems in general and battery production in particular.

Model coupling and co-simulation Co-simulation is a suggested method for the simulation of complex hierarchical systems and consequently usable for production systems or factories. This criterion refers to the combined use of different interdisciplinary simulation models within one application. The criterion is not fulfilled if only one model is used. The criterion is completely fulfilled if multiple models are individually implemented in the best-suited software environment and coupled via a coordinating middleware software.

Methodological contribution This criterion refers to the contribution of a publication to the methodology of multiscale production system simulation. This includes but is not limited to simulation methodology, model coupling, numerical aspects, and synchronization of data exchange. The criterion is not fulfilled if a publication does not address methodological issues towards multiscale simulation of production systems. It is completely fulfilled if methodological aspects are the main focus of a contribution.

Applicability This criterion refers to the application of existing simulation applications in an industrial production context. It is examined if models and tools are available and adaptable as well as if there are clear guidelines for application. The criterion is not fulfilled if a publication presents only a theoretical concept. The criterion is completely fulfilled if commercial software is used, executable models are developed, and guidelines or procedures for application are available.

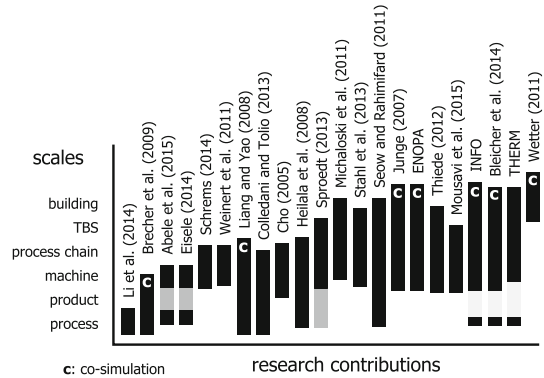
In addition to these criteria, all existing simulation contributions were analyzed regarding the used simulation approaches such as DE, AB, DS or SD.

3.2 Presentation and Evaluation of Existing Approaches

The presentation of research contributions begins with simulation applications addressing the smallest scales of a production system (processes, machines, products) and continues with simulations considering multiple and larger scales. All contributions are explained and discussed regarding the defined criteria. Figure 3.1 illustrates the identified contributions and the order of presentation based on the addressed scales.

While there are several applications and concepts in the field of battery cell and battery system simulation (e.g. Wieser et al. 2015; Allu et al. 2014; Du et al. 2014 and Yu et al. 2013), there are hardly any existing or established simulation approaches for individual processes of battery production. One of the few examples for process simulation is the simulation of different formulation strategies of the mixing process

Fig. 3.1 Qualitative structuring of identified research contributions in production system simulation regarding addressed scales



(Li et al. 2014). Furthermore, according to Kaiser et al. (2014), computational fluid dynamics are used for the dimensioning and design of coating devices. These simulations focus solely on processes without considering external influences such as machine interactions in an industrial production environment.

Outside of the research field of battery production, several simulation concepts focus on the combined simulation of processes and machines. For example, coupling of models is used to analyze the interactions between machining processes and related machine tools such as the impacts of vibrations or thermal effects on machining stability (Brecher et al. 2009; Aurich et al. 2009; Witt 2007; Schapp 2008). Many researchers work in this field which is called process machine interaction (PMI). An overview about research approaches in PMI is presented in Brecher et al. (2009). The majority of studies contains the analysis of machine structures, physical component behavior, process physics and interactions between machine, process and work pieces. These approaches focus on product quality and refer to small spatial and temporal scales of production systems.

Abele et al. developed a holistic simulation environment for the analysis of energy demands of machines by combining models for machine components and processes (Abele et al. 2012, 2015). They developed methods for the simulation-based assessment of the energy demand of machining processes for a given product geometry (NC files) and process parameters (e.g. cutting force). They combined models for machine, process, and product to simulate the resulting energy demand. This work was part of the research activity ECOMATION. In this context, Eisele (2014) developed a modular methodology and models for the simulation of machine components. Physical models for machine components (e.g. motor, valves, pipes, cooling system, etc.) have been summarized within a library (Simulink) which can be used for the definition of specific machines. These models also include process specific parameters. In a similar concept, Schrems (2014) proposed a machine simulation considering different machine components. The goal was to develop a method for modeling the energy demand of machine tools. The components of a machines with relevance to the energy demand are grouped according to their functions and demand behavior. Furthermore, he combined several machine models to simulate the energy demands

of an entire process chain (DE with Siemens Plant Simulation). He also suggested to identify the shares of each machine of the total energy demand as well as on the energy demand per product unit. Overall, this approach enables a detailed modeling of machines on component level aiming at the simulation of energy demands on process chain level.

The same goal was addressed by Weinert et al. (2011) who developed an energy block methodology for modeling state specific energy demands of machines on component level. Moreover, Weinert et al. extended the approach towards the modeling of multiple machines. This allows using the methodology to include energy related criteria into production system planning and scheduling. However, not much detail is presented about the implementation of the models.

Liang and Yao (2008) presented a hybrid modeling approach for production systems combining the tools Matlab/Simulink and Arena to determine continuous characteristics on process level and the discrete behavior of machines on workshop level. Arena was used to model production lines with multiple machines and to determine the output and waiting times per product type. Matlab Stateflow was used to describe the operational steps of machines. Matlab Simulink was used to imitate the process controller and to determine processing times and cutting forces for each work piece. ActiveX and VBA were used to control the continuous and discrete Matlab models through the DE Arena model. This approach enables evaluating the interactions between different scales of production lines. However, the specific target of the approach is not clearly stated. The output of products and cutting forces are calculated although it is not apparent how the results are used.

Colledani and Tolio (2013) developed an integrated multiscale and multilevel model for a material recycling system combining the process and process chain level. The goal was to estimate the performance of a de-manufacturing system considering the complex interdependencies between process physics (e.g. separation quality or size reduction) and the system dynamics (e.g. routing or utilization and profitability). However, the system dynamics analysis is not conducted by simulation but with analytic methods. Moreover, the physical process models refer to specific processes and seem not to be easily adaptable.

Cho (2005) developed a distributed simulation approach for the job-shop scheduling problem in which machines and parts are represented as events. The entities machine and part have properties and states and exchange information with each other via a developed communication architecture. The approach is able to determine the arrival time of parts for different machine allocations. However, the approach is targeted specifically to the scheduling problem, is implemented based on specific software solutions, and is not easily adaptable to other cases.

Heilala et al. (2008) developed an application which combines DE simulation and 3D modeling of production systems with LCA to perform a joint analysis of economic, environmental, and ergonomic characteristics of production systems. Their goal was to establish a simulation tool for supporting the production system planning phase. Their approach differentiates the higher level of product flow and the lower level of workstations and process steps. A DE simulation model is proposed for calculating the system performance (e.g. percentage of machine states, energy

demands) based on given schedules, product mix, product routes and other production characteristics. Furthermore, product properties are included since material properties and product dimensions have influence on economic and environmental performance indicators. They use software for integrated factory and robotic simulation (3DCreate and 3DRealize of Visual Components) and Excel for the calculation of related environmental impacts. A coupling of DE simulation and LCA calculation is suggested but not implemented.

Sproedt developed a similar concept which utilizes available life cycle inventory (LCI) data in combination with a DE simulation model in order to automatically generate LCA results for production systems (Sproedt 2013; Sproedt et al. 2015). The concept shall support the evaluation of improvement measures towards improving the eco-efficiency and the performance of production systems. He included modules for processes and supporting services in the simulation framework. These processes and supporting services are described by various parameters (e.g. processing time, MTTF) and states (e.g. idle, off, processing) which also include the behavior and characteristics of the related machines. An evaluation module allows the calculation of various results such as costs, throughput time, and environmental impact. The physical characteristics of processes and equipment are not modeled and the building environment is not considered. The approach is prototypical implemented and Sproedt further provided a detailed guiding procedure which supports the application of his approach for other production systems. A similar approach using DE simulation and LCA was presented by Löfgren and Tillman (2011).

The combined analysis of production operation and building energy management is motivated by Michaloski et al. (2011). They proposed the integration of manufacturing execution systems (MES) with energy management system (EMS) to identify and evaluate improvement measures towards energy efficiency and more sustainable production. The main idea is to use DE simulation to determine schedules of production activities including job and resource allocation, determine the production performance (e.g. utilization, scrap rate, product quality) and to link the production activities (e.g. based on average load profiles) to TBS (e.g. compressed air, HVAC). The focus is on identifying improved schedules of production activities. The authors provide their model structure and considered system elements as well as desired performance indicators for MES and EMS. However, they have published only few details about the DE simulation model and only qualitative simulation results.

Stahl et al. (2013) proposed a total factory simulation aiming at extending material flow calculation toward environmental goals. Their concept includes the state-based modeling of production assets such as machines combined with peripheral equipment. They generate power demand profiles of each asset depending on the asset's states. This concept was introduced to plant simulation.

Seow and Rahimifard (2011) proposed a framework for modeling energy demands on plant and process level from a product perspective. Their motivation was to determine the total energy required to produce one product unit and to derive optimization potentials for production operational as well as product design. They consider direct and indirect energy demands as well as theoretical and auxiliary energy demands. In order to allocate indirect energy demands to product units, they differentiate zones

of facilities with similar indirect energy demands. Their approach includes energy demands of TBS (e.g. compressed air, lighting, heating, process liquids) and auxiliary equipment which results in a multiscale perspective. They developed an integrated DE simulation model in Arena which allows to determine the embodied energy of product units of multiple product types. This is based on the simulation of the throughput of products through processes and different building zones. Product type specific processing times are implemented. The theoretical energy demands are calculated with mathematical models describing the characteristics of each process (e.g. based on specific cutting energy and volume of a parts). Auxiliary energy demands are estimated by equipment manufacturer specifications or determined by measurements but they did not include more detailed models of TBS system. Their tool can be used for what-if analysis of different scenarios. The authors clearly state that the generated results can be valuable input for further evaluations such as LCA or life cycle cost analysis. They further motivate to use the results as indicators for improvement potentials in product design. Multiple planning perspective are clearly addressed. However, the influences of processes on product quality are not considered.

Junge (2007) developed a method for the simulation-based development and optimization of energy efficient production control. The core of his simulation approach is a DE material flow simulation which enables to determine the energy demands and costs as well as the production costs and other logistical performance indicators (e.g. utilization, work in progress). Furthermore he modeled the current temperature, ventilation rate, and pollutant concentration inside a factory which are relevant conditions for the operation of machines and the calculation of costs for heating and cooling. This simulation model for the production system operation was coupled with a building simulation. A specific coupling solution was developed based on TCP/IP connections. The coupled simulation approach allowed analyzing the effects of different production strategies and schedules as well as to support the planning of TBS.

The goal of the research project ENOPA (engl.: Energy efficiency through optimized coordination of production and technical building services) was to develop an approach for the coupling of models for simulating energy demands of TBS and the building with a process chain in order to improve energy efficiency in production facilities (Hesselbach et al. 2008). The main motivation was to determine the timing of demands for different media (e.g. electrical energy, compressed air, hot water, or cooling liquids) of production processes and the resulting loads on supporting building equipment. A comprehensive summary of the project results can be found in the project report (ENOPA 2011) and in Hesselbach (2012).

Thiede developed a generic and adaptable DE simulation environment for analyzing the energy efficiency in production systems (Thiede 2012; Herrmann et al. 2011). He decided for an integrated modeling approach in order to avoid technical problems and synchronization issues arising from a coupling of models. The main goal was to assess the energy demands of production systems depending on the actual operation. The approach aims at supporting strategic and operational production management in the designs and control of production systems. For that reason, the simulation environment contains generic modules for processes and TBS (e.g.

compressed air and steam generation). This allows to determine the load profiles for all observed energy carriers of the relevant equipment within a production system in order to identify hot spots and peak loads. The process modules and the sub-models for TBS are integrated within one model which is implemented with the software AnyLogic. The model is flexible, modular, and scalable to be usable for different industries. The simulation environment was used to demonstrate what-if analyses for different scenarios of improvement measures. For example, the approach allows changing operational system parameters (e.g. production speed) and to determine the total energy demand.

Mousavi et al. (2015) presented a modeling approach for the integrated evaluation of energy demands of unit processes and the entire production systems. The goal of their energy-oriented factory simulation is analyzing the impacts of specific machine tool parameters on the energy demand on production system level. They proposed a framework which divides process chains into different unit processes which are characterized by machine specifications, the design of products and the related process. The process chain is supplied by peripheral and TBS equipment. Their approach can determine the total time-dependent energy demand of the production system as well as indicators describing the production performance such as lead time and output. Within their implemented hybrid simulation model, they integrated models for unit processes with models for TBS and a process chain model which is controlled by a production control unit. They presented two case studies showing that the lot size and machine parameters have impacts on the energy efficiency of the entire system.

The project INFO (Interdisciplinary research for energy optimization in production operations) pursued the similar goal of increasing energy efficiency in production by using a holistic factory simulation. More specifically, the goal was to obtain a holistic contemplative simulation model to investigate the energy and resource efficiency of production facilities already within the planning stage (Dür et al. 2013). The main objectives were the analysis and reduction of the energy demand as well as the related CO₂ emissions and the economic profitability. That means that economic and environmental goals are simultaneously addressed. For this purpose, the INFO approach integrates the disciplines of power engineering, production technology and building design. Within this project, several researcher worked on different aspects of such holistic factory simulation. Leobner et al. (2011) presented an overview of components of production facilities (structured in physical and information components) as well as related rules, parameters, boundaries, and interfaces of interactions which should be considered in a holistic modeling approach. Hafner et al. studied the practicability of co-simulation with BCVTB for simulating the thermal processes in a production building with the goal to optimize the energy usage in cutting factories (Hafner et al. 2012, 2014). They coupled models for machines, the energy system, and a building with different zones. Machines are modeled in Modelica, Simscape and Matlab (simple data model combined with MS Excel). Machines in Dymola and Simscape are simplified represented by electrical motors at which electrical energy is lost at the resistor and converted into thermal energy (heat flow to the building). Kovacic et al. (2013) further discussed the potential benefits of coupled simulation based on a parametric simulation case study including a

life cycle cost analysis of a production facility with a focus on the building. Heinzl et al. (2013) set a research focus on the communication, step size, and synchronization methodology of simulation models. He used an energy system model (Modelica) and a building model (EnergyPlus) to evaluate different production scenarios and building locations regarding the electrical power demand. The complete project results are presented in Dür et al. (2013). On machine level, machines are represented as parameter models based on state specific average energy demands (although physical machine models were presented for example by Hafner et al. 2014). Parameter models were implemented for machine tools, compressors and lasers. Building models were created in EnergyPlus but further simulation studies were also conducted with COMSOL multiphysics (2D) CFD-simulation for evaluation of influences of temperature distribution on the energy demand. BCVTB was used to combine Matlab, Excel, EnergyPlus, and Dymola. In summary, all relevant aspects of production systems related to energy flows were addressed at different levels of detail. However, traditional production objectives such as utilization, availability, lead time or throughput were not part of the analysis. The simulation does not include a specific model for a process chain. Furthermore, a product perspective is missing and process physics with respect to product properties are not part of any simulation sub-model.

Based on results from the INFO project, Bleicher et al. (2014) further presented a prototypical simulation framework and exemplary models for supporting the planning of production facilities by combination of specialized simulation models for production equipment, energy system, and the building. Machines are represented by multi-domain models combining electrical, mechanical, and thermal aspects of machine tools. As an example they have presented a model of a turning lathe drive train. The software Matlab Simscape is used to model the energy flows. These models do not include operational machine characteristics such as availability, capacity, or MTTF. Also the authors state that models become increasingly complex if multiple machines have to be simulated. They suggest the use of energy demand profiles based on empirical studies to substitute physical models. Their models are reduced to relevant energy related states with allocated average energy demand. Using the detailed physical models is suggested for validation and prediction of energy demands outside the co-simulation. The operation of machines (e.g. scheduling and job allocation) is controlled by production data which in the presented case was retrieved from SAP. The actual material flow of products through multiple machines is not simulated. Furthermore, the value adding physical processes and their influence on product characteristics are not included in their models. Consequently it is not possible to evaluate performance indicators such as lead times or quality rates. The energy system and related equipment is included in the co-simulation. The compressed air generation is also mentioned in the case study but it is only stated that the power demand of the compressors was represented with a physical model. The building is said to be modeled within the software EnergyPlus according to the building information modeling (BIM) methodology. However, no detailed information is given about the energy system model, compressed air system model, or building model. Furthermore, it is not explained how the static parameter models are linked with simulation models.

A similar objective was addressed in the project THERM (THrough-life Energy and Resource Modeling) which aimed at reducing energy demands, carbon emissions and waste through integrated simulation of production operations and building environments. The main result is a sustainable manufacturing modeling tool of which the requirements, the model concept, the graphical representation, and the prototypical implementation are presented in various publications (Wright et al. 2013; Despeisse et al. 2012, 2013; Oates et al. 2011; Ball et al. 2013). The authors found that existing physical building simulation tools did not allow to sufficiently consider heat emissions from production equipment into the building environment (Oates et al. 2011). As a result from this, they proposed a combined simulation of the building environment, production equipment, and supporting TBS in order to determine the heat balance and energy flows in a factory. The prototypical THERM simulation tool and the defined workflow enable modeling of the climatic environmental conditions within a factory building and the interactions with production equipment depending on operational states. The tool is based on IES Virtual Environment. It enables the determination of the total energy demand of a production facility and the evaluation of improvement measures such as the reuse of resources. Moreover, a set of predefined improvement measures (tactics) is provided. Ball et al. further proposed integrating the effects of resource flows (e.g. parts, material) through a factory. However, the tool includes neither the evaluation of traditional production performance indicators nor product properties or detailed process and machine behavior. Also, no detail information is given about how the energy and resource flows are actually modeled and how or if different schedules for equipment operations and jobs are considered.

Outside the field of production simulation, the simulation of buildings and building controls are broadly covered topics in building engineering and simulation science. In this context, various multiscale and co-simulation approaches were developed addressing the interactions between different building elements (e.g. Trčka et al. 2010; Wetter 2011; Sagerschnig et al. 2011; Wills et al. 2012; Zhang et al. 2013). Many of these approaches focus on the integrated analysis of the interactions between building shells and HVAC systems. Trčka and Hensen (2010) provide an overview of related simulation approaches. As an example of a simulation concept, Chen et al. (2015) used co-simulation to study the interactions between indoor climate in a multi-zone building and energy efficiency measures.

To summarize the results of the evaluation, Harvey balls are used to represent the rating of the evaluation criteria. Harvey balls indicate the degree to which a research contribution fulfills the related criteria.² The results of the comparison are shown in Table 3.1. It must be emphasized that the results were also significantly influenced by the type and level of detail of the publications.

The table shows clearly that no simulation concept fulfills all criteria which are relevant for the desired multiscale simulation of battery production systems.

²A white empty ball (○) indicates that a criteria is not fulfilled at all while a black filled ball (●) indicates that a criteria is completely fulfilled. Partial fulfillment of a criterion is indicated by partially filled balls (◐, ◑, ◒).

Table 3.1 Evaluation of research contribution

	Li et al. (2014)	Brecher et al. (2009)	Abele et al. (2015)	Eisele (2014)	Schrems (2014)	Weinert et al. (2011)	Liang and Yao (2008)	Colledani and Tolio (2013)	Cho (2005)	Heilala et al. (2008)	Sproedt (2013)	Michaloski et al. (2011)	Stahl et al. (2013)	Seow and Rahimifard (2011)	Junge (2007)	ENOPA (e.g. Hesselbach et al. (2008))	Thiede (2012)	Mousavi et al. (2015)	INFO (e.g. Dür et al. (2013))	Bleicher et al. (2014)	THERM (e.g. Wright et al. (2013))	Wetter (2011)
Scope																						
Battery production relevance	●	●	●	●	●	●	●	○	●	●	●	●	●	●	●	●	●	●	●	●	●	●
Multiple planning perspectives	○	○	●	●	○	○	○	●	●	●	●	○	○	●	●	●	●	●	●	●	●	○
Integrated objectives	○	●	●	○	○	○	○	●	○	○	●	○	○	○	●	●	●	●	●	●	●	○
Production system scales																						
Process	●	●	●	●	○	○	○	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○
Product	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Machine	●	●	●	●	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Process chain	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
TBS	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Building	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Methodology and application																						
Model coupling and co-simulation	○	●	●	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Methodological contribution	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
Applicability	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○

3.3 Findings and Research Demand

The evaluation has shown that there is a diversity of simulation concepts and applications which were developed for various purposes addressing different goals and planning perspectives. It has revealed that the idea of a multiscale factory simulation may provide various advantages but no published simulation concept was found which fulfills all criteria relevant to the desired multiscale simulation of battery production. The majority of developed simulation concepts were designed for discrete

production scenarios which allows an adaptation to battery production. Some concepts also include aspects relevant for a multiscale simulation of battery production, such as the combined analysis of production activity and TBS. However, only very few simulations directly address battery production (e.g. Li et al. 2014).

Furthermore, none of the reviewed simulations supports all planning perspectives. Some simulations aim at supporting operational and tactical decisions such as the combined evaluation of schedules and production system configuration (e.g. ENOPA). Other simulations allow the evaluation of production system performance combined with strategic planning tasks such as LCA (e.g. Sproedt 2013), factory planning (e.g. INFO) or product design (e.g. Seow and Rahimifard 2011).

The review has also shown that coupled or integrated simulation approaches either consider larger or smaller scales. Simulations linking the modeling of the building and TBS with production operations in general simplify the process and product scale and use abstract models of machines. Simulations considering the process physics or product states and traditional production objectives within a process chain usually do not consider the building environment or TBS in greater details. Overall, no simulation application combined detailed models for all scales.

In addition, the results show that only very few simulation concepts address methodological issues regarding the application of coupled or co-simulation for production systems. No publication was found in the context of production system simulation which provides a defined framework for structuring simulation models, a definition of relevant system parameters, state variables, and variables for data exchange between models. The only concept aiming in this direction was published by (Leobner et al. 2011) who defined the relevant system elements but without specifying how these elements has to be modeled and which information has to be exchanged. Wetter (2010) present detailed concepts for co-simulation in the context of building simulation which could be transferred to production system simulation.

Similar, no reviewed simulation concept allows an integrated evaluation of technological, economic, and environmental objectives. The majority of the found simulations address the energy demand of production equipment and consequently – since energy contributes to the production costs – a combined evaluation of economic and environmental objectives. Only very few simulations aimed at the evaluation of the product quality in correspondence with process parameters (e.g. Brecher et al. 2009 and Li et al. 2014) but they neglect economic or environmental objectives. And although the idea of PMI is transferable to battery production (and in particular to cell production), the reviewed simulation concepts (e.g. Witt 2007) focused on machining or forming processes which is of limited relevance for battery production.

Furthermore, the reviewed simulation applications show no evident structure regarding the relations between the addressed objectives (economic, environmental, quality), production system scales (product, process, machine, process chain, TBS, and building) and the used simulation approaches (DE, DS, AB, SD, and co-simulation). This information would support developers of multiscale simulation in selecting the best suitable simulation approach for their objectives. Figure 3.2 presents these findings by showing the research contributions on the left, simulation approaches on the right at the top, objectives on the right in the middle, and scales on

the right at the bottom. The lines indicate the relations and the line color is inherited from either the simulation approaches, objectives, or scales. The figure shows that DE and DS are the dominating simulation approaches whereas DS is mostly used for simulations considering low or high production system scales. DE is used in most of the simulations except for the lowest or highest scales. Co-simulation is not often used and only applied in simulations considering small or large scales. Economic and environmental objectives are equally often addressed while product quality is neglected in most simulations. Accordingly, the product scale is not considered in many simulations. It can be seen that the lines from different scales do not intersect very often. Since the contributions are ordered from small to large scales, this means that simulations mostly address only one or few different scales. The figure shows that the scales machine and process chain are most considered. Overall, most

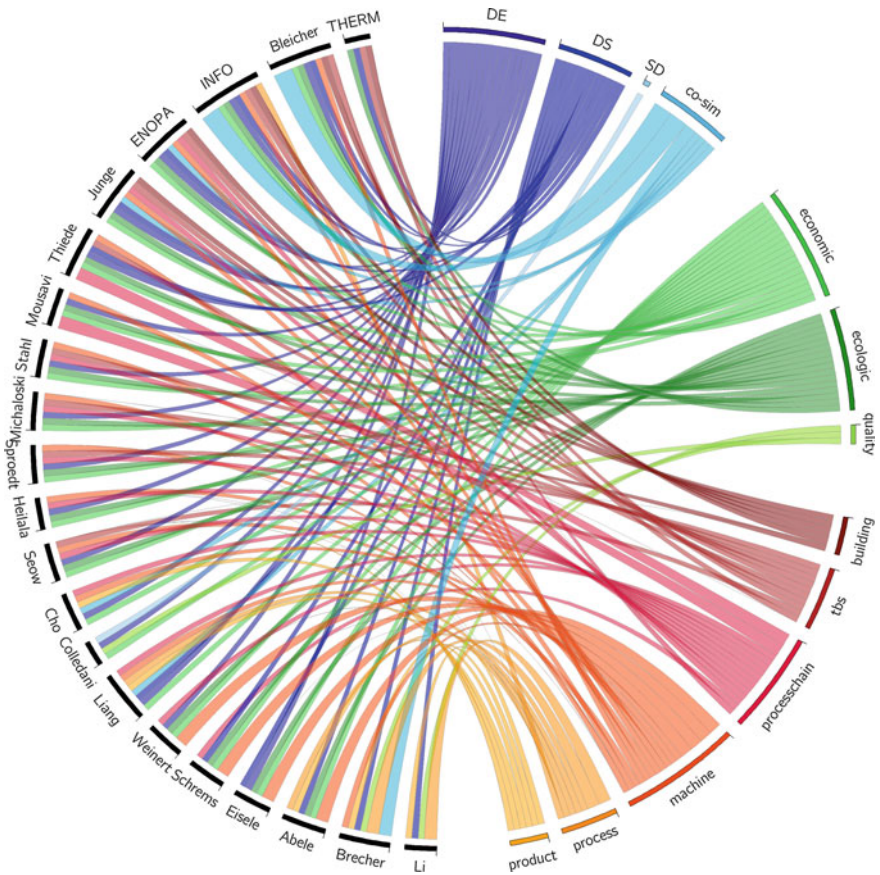


Fig. 3.2 Radial chart of the connections between research contributions, objectives, simulation approaches, and addressed scales of production systems

of the reviewed simulations use DE and DS simulation to address economic and environmental objectives by considering interlinked machines.

Although the reviewed research contributions provide various relevant concepts and modeling solutions for production system simulation, there is still further research demand towards the desired multiscale simulation of battery production systems.

In this context, the most relevant demand refers to the **combination of a detailed multiscale co-simulation of a production system** including TBS and the building (e.g. as in project INFO or Bleicher et al. 2014) **with a process chain simulation** (for different process chain configurations, such as in Thiede 2012) for the coordination of machine operation in interaction with TBS. The machines within such process chain model must be modeled in greater detail (e.g. as in Abele et al. 2015 or Weinert et al. 2011) to be able to evaluate the influence of different machine parameters or configurations on system level. The process chain model must further be able to evaluate traditional production objectives such as throughput time and output. This is important for the evaluation of economic objectives and so far neglected in detailed co-simulations which focus mostly on energy demands.

Furthermore, a stronger emphasis has to be put on the **product perspective**. The product quality must be included in a multiscale simulation. For this reason, it must be possible to describe the influences of processes on characteristics of product units. This requires detailed physical process models or simplified parameter models (see Brecher et al. 2009) which determine the process results for each product units based on product type specific process parameters. These process models – or co-simulations combining models for processes and machines – must be connectable to the process chain model to get information about the required processing of a specific product type. Moreover, the evaluation of the product quality along the process chain is of great interest. For this reason it must be possible to trace the characteristics of each product units through the process chain. This feature was not found in any of the reviewed process chain simulations. It requires product units to be individual entities and not just events as in DE simulation. In addition to the tracking of product characteristics, it should be possible to determine the specific demands of materials and energy for each product unit (similar to Seow and Rahimifard 2011). This fosters the evaluation of environmental impacts.

Multiple planning perspectives can be addressed by a **modular model structure** in which sub-models can be exchanged or added in order to achieve suitable results for operational, tactical, or strategic planning tasks. At an early planning stage, models must not be too detailed but operational decisions may require very accurate results in high resolution. In this regard, co-simulation seems promising for creating a modular structure. However, required is a framework for structuring the different models as well as guidelines for model specification and co-simulation design.

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Chapter 4

Multiscale Simulation Modeling Concept for Battery Production Systems

The purpose of a multiscale simulation of battery production systems is enabling an integrated evaluation of improvement measures regarding production costs, product quality, and environmental impacts, as well as gaining interdisciplinary system understanding. Figure 4.1 illustrates how different disciplines can use a multiscale simulation to evaluate their specific improvement measures virtually and receive results indicating the related impacts on system level.

This chapter covers the development of a multiscale simulation concept for battery production systems which is the basis for a later implementation of such simulation within software. The goal of this concept is supporting the development of a multiscale simulation and to develop specialized simulation models considering the required inputs and outputs for the use within the multiscale simulation. The review of the state of research has shown that such concept is not available but that the demand for multiscale production simulation is strong. The resulting research demand and the motivation for a detailed analysis of battery production systems led to a set of objectives for the desired simulation concept (Sect. 4.1). Based on the identified objectives and derived requirements, the simulation concept was developed by defining the system boundaries and a model framework (Sect. 4.2), describing the content and logic of the identified relevant models (Sects. 4.3 and 4.4), selecting suitable model coupling strategies and variables for data exchange (Sect. 4.5), and defining the achievable results (Sect. 4.6). Finally, an application procedure is suggested which describes how a specific multiscale simulation could be developed (Sect. 4.7).

4.1 Objectives and Requirements

In general, objectives (O) describe what should be achieved and requirements (R) describe what has to be done to fulfill the objectives. The derivation of objectives was

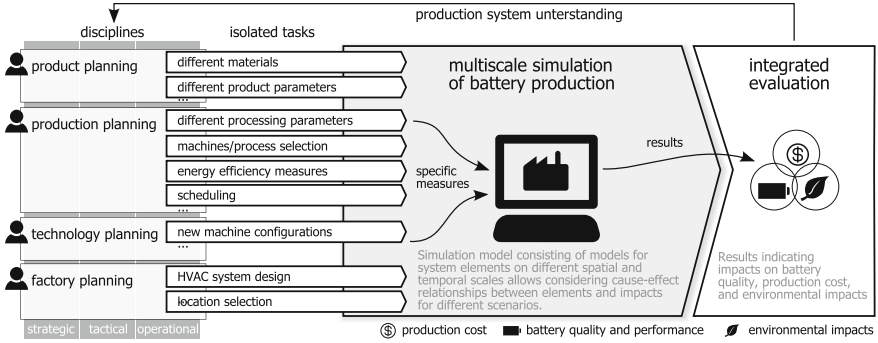


Fig. 4.1 Scheme of a multiscale simulation of battery production systems

based on a deductive approach and the identified objectives were transformed into specific requirements for the multiscale simulation. The objectives and requirements are grouped according to the topics simulation structure, simulation objectives, model architecture, model specification, and cooperative employment.

Simulation Structure

The main objective of this simulation concept is providing the theoretical foundation for the development of a software-based multiscale simulation environment. The concept has to define the fundamental structure of the simulation approach which has to be flexibly applicable to different configurations of production systems for different product types [O₁]. The simulation must be usable for electrode and cell production (independent of a specific cell type such as LIB or next generation cells) as well as for module and system assembly [O₂]. Also it has to consider multiple goals for the improvement of these production stages [O₃]. These superordinate objectives lead to the following requirements.

- R₁** Definition of system boundaries of the simulation approach regarding content of the simulation, desired results, and use cases.
- R₂** Definition of production system elements which are required for integration into the multiscale simulation.
- R₃** Elaboration of the spatial and temporal scales required to represent the behavior and interactions of elements within the hierarchical structure of production systems according to the desired results.
- R₄** Formation of a framework for clustering of models for production system elements and information flows between models considering the hierarchy of production systems.
- R₅** Realization of a flexible model structure to model all production stages.

Simulation Objectives

The simulation approach targets the interlinked improvement of production costs, product quality, and environmental impacts of batteries and their components [O₄].

These tasks depend on the derivation and simultaneous evaluation of improvement measures. The simulation shall support these tasks by creating transparency about the production system behavior [O₅]. This requires the

- R₆** definition of production stage specific performance indicators for technological, economic, and environmental evaluation, as well as the
- R₇** derivation of state variables and parameters of simulation models needed for the calculation of the defined performance indicators.

Model Architecture

Based on these indicators and variables, the concept has to specify the functionality of the multiscale simulation environment in alignment with the involved models and desired simulation results [O₆]. This requires the

- R₈** selection of required models for the detailed simulation of production system elements, and the
- R₉** detailing of all models regarding their inputs and results as well as the inherent model type (e.g. empirical vs. physical) and logic.¹

Model Specification

It is necessary to specify the simulation models in order to get desired results. This includes the model functions for the evaluation of traditional economic production objectives and environmental impacts [O₇]. This leads to the following required functions of a multiscale simulation.

- R₁₀** Simulation of material flows of jobs through a process chain.
- R₁₁** Characterization of finished jobs by production time, used resources, date and time stamps, as well as value adding and non-value adding time shares.
- R₁₂** Consideration of blocking, starving and machine failures to imitate a realistic system behavior.
- R₁₃** Simulation of energy demands of all equipment based on load profiles which enable determining environmental impacts related to energy generation as well as energy costs.
- R₁₄** Simulation of used quantities per material type and amount of scrap materials for calculation of material costs and the amount of used and wasted materials.

Moreover, the simulation shall enable identifying the relevant product characteristics and product specific influences on the production system [O₈]. Also it should allow the analysis of cause-effect relationships between processes and product characteristics (e.g. process tolerances) along a process chain [O₉]. This requires:

- R₁₅** a product model which allows tracing the product characteristics of semi-finished work pieces and products during production (this has to include product specifications, the current state of production, and product characteristics).

¹The logic refers to the characteristics of the modeled element as well as the type and structure of relations between parameters, variables, and performance indicators (e.g. equations or parameter-based relations).

R₁₆ product instances to have individual values for characteristics to enable the analysis of deviations of characteristics (this is needed to store information about process tolerances and the effects on product characteristics).

R₁₇ the definition of product type specific process routing and required processes.

In order to analyze cause-effect relationships and trade offs, it is important to simulate the interactions between the production system activities and the operation of installed equipment along with the specifications and the characteristics of products [O₁₀]. The simulation must enable to perform different experiments to evaluate the impacts of improvement measures, product designs, and production strategies on system level [O₁₁]. The results of these experiments have to be easy to interpret and to create transparency about the system behavior. This requires

R₁₈ multiscale modeling of effects and relations between machines, auxiliary equipment, TBS, and the environment inside a building.

R₁₉ a process chain model to determine the activity in a production system.

R₂₀ adaptable simulation periods to identify effects on different temporal scales.

R₂₁ adjustable model parameters to define specific production system scenarios.

R₂₂ visualization of variables and performance indicators over time.

R₂₃ specific report layouts for different performance indicators and stakeholders.

Cooperative Employment

The simulation concept shall facilitate the cooperation of experts from different domains and disciplines by combining their knowledge into one simulation approach, based on specialized models [O₁₂]. The concept has to provide guidance on how a multiscale simulation environment has to be developed, employed, and maintained [O₁₃]. Moreover, the concept has to be independent from a specific software or model implementation [O₁₄]. This requires

R₂₄ a definition of the information exchange and interfaces between models (regarding required inputs from and outputs to other models).

R₂₅ knowledge about model coupling in the context of production systems.

R₂₆ a procedure for the development and employment of a multiscale simulation including the development of each suggested model type.

The presented objectives and requirements for the multiscale simulation concept are the starting point for the modeling framework development and the specification of individual models.

4.2 Modeling Framework Development

The purpose of the multiscale modeling framework is supporting the selection and structuring of simulation models based on defined system boundaries of the simulation as well as on the hierarchy and scales of battery production systems.

4.2.1 *System Boundaries and Scope*

The definition of system boundaries and the scope of the simulation is an important prerequisite for determining the simulation content, the model inputs and outputs, the simulation goals and desired results, as well as the involved stakeholders. System boundaries define which aspects of battery production have to be included in a simulation and the scope describes the challenges and related planning tasks.

The starting point of the definition of system boundaries and associated scope is the analysis of the production stages of battery production: electrode and cell production as well as module and system assembly (see Sect. 2.1.3). The production of electrodes and cells involves chemical and physical processes in a defined sequential order but without an uniform tact time due to a large spread of processing times. The order of processes is identical for all product variants and the number of electrode or cell variants per process chain is low. The processes need specialized machines and peripheral equipment for media supply or to maintain particular ambient conditions (e.g. temperature or humidity). The major challenges in cell production are the selection of suitable equipment, identification and evaluation of cause-effect relationships between processes and product quality, determination of optimal process parameters, analysis of energy efficiency measures, as well as the elimination of bottlenecks in order to achieve a full utilization of expensive resources.

The module and system assembly consists of various automated or manual handling and assembly tasks which can be very different depending on the design of modules and systems. In contrast to the rather predefined production of electrodes and cells, there are many possible sequences for the assembly of modules or systems (Li et al. 2011). And due to a high product variety, the sequence of processes can be different for each job. Consequently, the material flow of jobs through the assembly system is not predetermined and can be subject to optimization regarding a short tact time. In contrast to electrode and cell production, there are no strict requirements regarding building ambient conditions. The influences of the actual processes on product quality is relatively low compared to the influences of processes in cell production. However, the characteristics of the used cells also determine the performance of an entire battery system. This leads to the necessity to also consider product characteristics in the assembly of modules and systems. This also allows using simulation to evaluate selective assembly strategies, which aim at combining most compatible cells into one module (Schmitt et al. 2014).

The planning tasks differ for cell production and system assembly. While in the first the focus of improvements lies on product quality, energy efficiency, and resource utilization, the focus in the second lies on achieving a high assembly system utilization and reduced throughput times while handling a high product variety with high volumes. High product variety is a challenge if variants require different processing times for the same production steps. Hence, the line balancing problem is more relevant in the module and system assembly as it is for electrode and cell production. These different improvement goals lead to the conclusion that it is

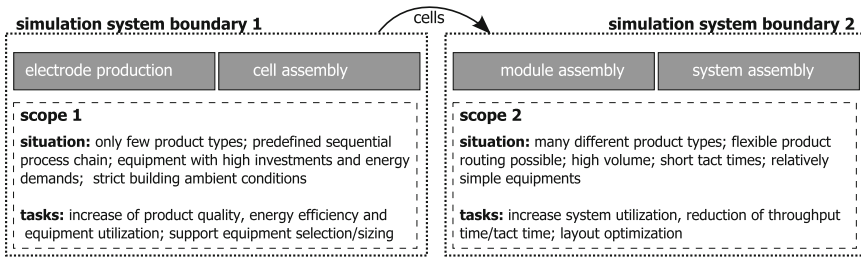


Fig. 4.2 System boundaries and scope

reasonable to differentiate system boundaries for cell production and battery system assembly. Figure 4.2 summarizes the system boundaries and the respective scope.

4.2.2 Hierarchy and Scales

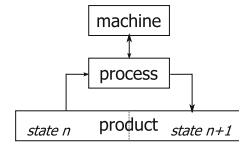
The system boundaries determine the battery production system elements which have to be included in a multiscale simulation. In addition, the framework needs to incorporate the hierarchical structure of these elements and their associated scales in order to specify the required flows of information between simulation models.

The existing hierarchy concepts (see Sect. 2.1.2) use different levels for their description of a production system which represent different scales. Spatial scales refers to the size and geometrical extend of a production system element as well as to the organizational allocation and relations of system elements. As an example, a production machine is on a smaller spatial scale compared to a process chain or the factory building. A machine is also part of a process chain and a process chain is contained in a building. Another example is the allocation of TBS to single or multiple machines, a process chain, or the building. TBS are on larger spatial scale than the machines but on smaller scale than the building.

In addition to spatial scales, the hierarchical framework for simulation models has to consider different temporal scales since the response time and the relevant evaluation periods differ for various system elements. Consequently, it is necessary to derive the framework based on relevant spatial and temporal scales.

The main activity of production systems is creating products which is in general described by input-throughput-output processes. Batteries and battery components require many processes which transform a current product state to the next desired state by using machines, energy, and material. Machines, processes, and products are the elements on the smallest spatial and temporal scales of a production system. This means that the smallest value adding unit within a production system consists of a machine, a processes, and a product. This unit is illustrated in Fig. 4.3. A product is transformed from product state n to state $n + 1$ by a process which is defined

Fig. 4.3 Smallest value adding unit of a production system



and characterized by process parameters. A machine is used for the execution of the process.

The combination of processes and related machines to process chains represents the second spatial scale. Regarding the temporal scales, the duration of single processes usually ranges from seconds to hours. The production of one product can take hours and the production of multiple products (e.g. of a job with a specific quantity of product units) can be measured in hours or days. The operation and performance of process chains or multi-machine environments depends on schedules and the production program which are valid for days, weeks, or months.

On higher scales, TBS can be differentiated between building related services (e.g. energy supply, ventilation, or lighting) and process related services (e.g. compressed air supply).² For this reason, TBS are allocated to a spatial scale between process chains and the building shell. Regarding the temporal dimension, TBS cover a larger time spectrum. The interaction of TBS with processes has to be analyzed within intervals of seconds. The energy supply peak load is determined for intervals of 15 min. Temperature and humidity in a building change continuously but relatively slowly within hours creating heating, cooling, or dehumidification demands. The demands of processes (e.g. compressed air or air suction) can vary depending on the utilization of the production systems which can change during weeks or months. Thus, TBS systems have to be observed on different time scales.

The building is on the largest spatial scale of a production system. It contains all equipment and products and is exposed to the outside environmental conditions such as temperatures or humidity. These conditions depend on the season and the location of a building. The relation between the outside conditions and the inside ambient conditions is influenced by the building construction and the operation of HVAC systems. Consequently, the energy demands of HVAC systems depends on the outside conditions and its analysis requires a larger time scale in order to account for seasonal effects. Figure 4.4 illustrates the arrangement of production system elements within the spatial and temporal scales.

The structure of spatial and temporal scales is the foundation for the framework which defines of relevant simulation models within a multiscale simulation and their interactions within the defined system boundaries.

²Sometimes the term TBS is also used equivalent to auxiliary equipment of machines such as a decentralized cooling system. This equipment is directly related to single machines and not allocated to TBS. It is suggested to be included within the modeling of the related machine.

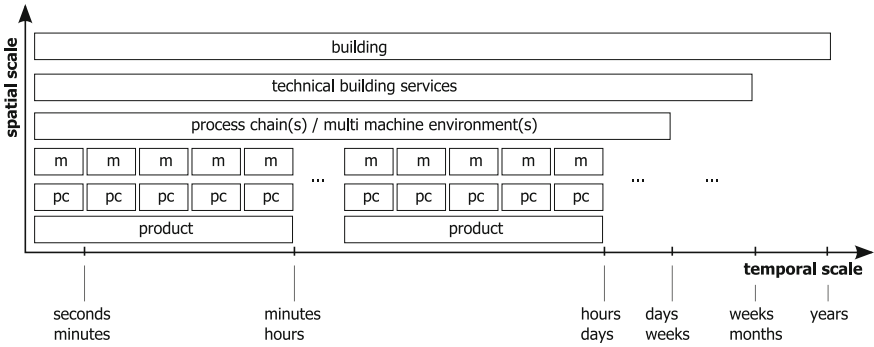


Fig. 4.4 Spatial and temporal scales of production systems (pc: process, m: machine)

4.2.3 Multiscale Model Framework

The framework clusters models for production system elements, defines interfaces, and proposes a lean flow of information between models. It has a generic character which allows using it as a foundation for multiscale simulations for any type of production systems. Consequently, it can be used and adapted for both the production of cells and the assembly of modules or systems. Figure 4.5 illustrates the framework which consists of layered model categories, exemplary model instances, and indicated information flows. The most upper layer – containing models for machines, processes, and intermediate or final products – represents the smallest spatial and temporal scale of a production system. While going to lower layers of the framework, the spatial and temporal scales increase according to the arrangement in Fig. 4.4. Machines are part of a process chain and operated by workers. The process chain model is the core of the multiscale model structure and it describes the material flow within a multi-machine environment. Furthermore, it coordinates the information flow between models on different scales. A process chain is supplied by machine related TBS. Other TBS are related to the operation of the building and models of these TBS system interact with the building model on the lowest framework layer.

The models are embedded in an infrastructure for model coupling which provides the interfaces and data sources required by the models to interact with each other. Inputs into the framework are data needed for developing and configuring the individual models. Examples are data about machines (e.g. energy demands), product bills of material, routing of products, machine allocation, or the construction of the building. Outputs of the multiscale simulation are diverse results which have to be evaluated and visualized.

The following chapters describe the different elements of the multiscale simulation framework in the order indicated by the numbers in Fig. 4.5.

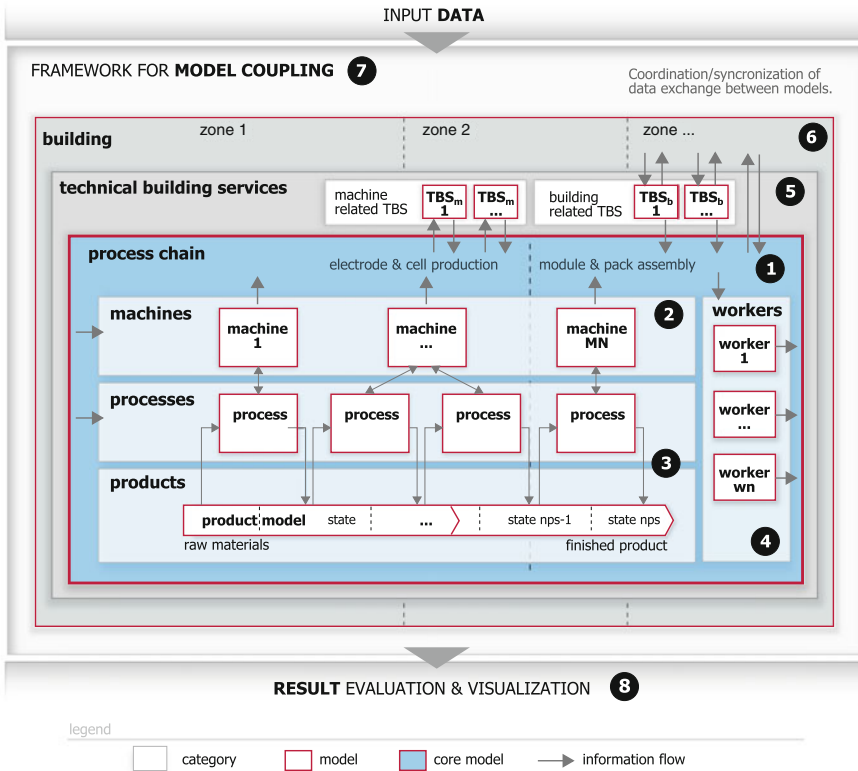


Fig. 4.5 Framework for multiscale simulation of production systems

4.3 Process Chain Model (1)

The process chain model imitates a multi-machine environment and acts as the coordinator of product specific production activities. One function is determining the schedules of machines and the routing of jobs through the production system in order to derive demands for TBS as well as the related effects on the building environment. For this purpose, it gathers and aggregates information from all machines to determine demands for supplying units such as related TBS. More specifically, the model represents the operation of machines to consider their availability, aggregate the values of state variables of machines (e.g. power demand), to generate performance indicators, to incorporate different production strategies and product routing, and to coordinate the flow of product units between machines according to machine allocation and schedules. With these functions, the model imitates the dynamics on the “shop floor” by coordinating the system elements according to the production program and defined production rules. The model further allows to examine the movement of product units for tracing product characteristics and the impacts

of different product types and production activities on performance indicators (e.g. utilization, energy demands). Furthermore, the model collects information and acts as a hub for information exchange with other models.

4.3.1 Process Chain Elements

The process chain model, based on an object oriented approach, allows modeling of a process chain which consists of a number mn of machines or workstations³ $MACH_{mn}$, each with a buffer B_{mn} with buffer capacity bac_{mn} . Machines are located on a virtual shop floor according to a defined layout. The process chain can be configured to produce a number ptn of different product types PT_{ptn} such as variants of anodes, cathodes, or cells. The production of each product type needs a finite sequence of production steps (PS_{ptn}). As an example, the production of an anode requires the production steps mixing, coating and drying, calendaring and separation. Hence, the production steps indicate the sequence of required processes⁴ where nps_{ptn} is the total number of production steps of product type PT_{ptn} ($PS_{ptn} = \{PS_{ptn,1}, PS_{ptn,2}, \dots, PS_{ptn,nps_{ptn}}\}$). Each production step has to be assigned to at least one machine. Vice versa, the available machines must be able to perform all production steps of all product types. The allocation of production steps to machines may depend on the machine configuration, dimensions or work space, tools, and peripheral equipment. The allocation determines the routing of a product units through the production system during production.

The routing of product units during production is different for batch or single unit production. Batch production means that an entire job J_{jn} (with job number jn) is produced on one machine simultaneously or until all product units of the job are done with processing. A flow of single product units means that the first product unit of a job is forwarded to the next machine as soon as it is done with processing. The second product unit starts processing as soon as the first leaves the machine. A job is finished if all product units have completed all production steps. Combining batch and single product flow within one simulation is not common since – in traditional DE process chain simulation – the flow of same types of entities (batches or single product units) is usually represented by occurring events. However, battery cell production contains batch and single unit processes. Consequently, the process chain model must be able to simulate the flow of batches and single product units as well as diverging and converging flows. For this reason, so-called processing units PU_{pun}^{ptn} are introduced to the process chain model. Processing units are characterized by a

³The term workstation is used if no specific dedicated machine is utilized for a production step. This might be the case in assembly systems relying on manual labor. It is usually not the case in fully automated series production.

⁴The differentiation between production steps and processes is proposed since same processes can be required multiple times for the production of a product type but with other process parameters and utilized machines. A described sequence of production steps avoids confusion about which specific processes are actually required.

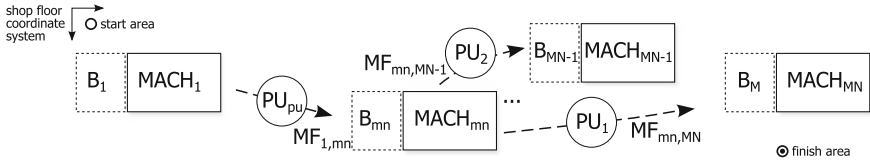


Fig. 4.6 Process chain structure with machines (MACH), buffers (B), material flows (MF), and processing units (PU)

number *pun* and an associated product type (*ptn*). Processing units can represent batches or single product units and they are the modeled entities which actually move to machines during simulation until all related production steps are completed. Using processing units allows modeling the flow of a batch from machine to machine (as one processing units) as well as the individual flow of several product units (as several processing units) related to one job. This model structure makes it possible to utilize multiple machines simultaneously by processing units related to one job which reflects a realistic system behavior. Figure 4.6 shows an exemplary process chain configuration consisting of machines with buffers and processing units with the related material flows $MF_{cmn,nmn}$ from the current machine (number of current machine *cmn*) to the next machine (number of next machine *nmn*). Each material flow is characterized by distance and velocity of the transport of a processing unit between two machines.⁵

For each job which has multiple assigned processing units, it has to be specified which processing unit has to be finished before a consecutive processing unit can be created. For example, in battery production electrodes are produced in batches. The resulting semi-finished product after these processes is an electrode coil from which electrode sheets are cut out. So far, an electrode batch can be represented by one processing unit. Next, a number of anodes and cathodes are used to create a cell. Each cell of a job individually travels through the machines until completion. Each cell is represented by one processing unit. Overall, a job of a specific quantity of cells starts with the batch production of electrodes and finishes when the last cell is completed. During system assembly, a number of cells is used to assemble a module and a number of modules is used to assemble a system. Figure 4.7 shows the relations of processing units for the stages of battery production. The routing of these processing units depends on the allocation of production steps to machines, the configuration of the process chain, and the selected control strategy.

⁵The possible velocity depends on the product type (e.g. size, weight), handling equipment and conditions such as obstacles (e.g. doors, air locks, slopes). The distance depends on the machines locations within a defined shop floor coordinate system.

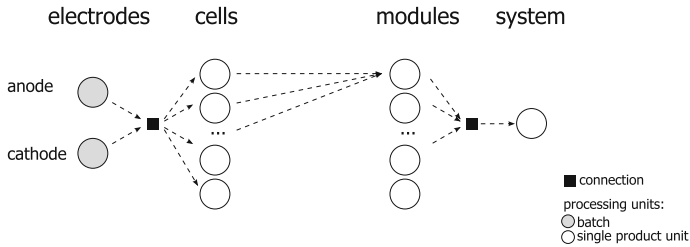


Fig. 4.7 Structure of processing units for cell production and system assembly

4.3.2 Process Chain Configurations and Control Strategies

The process chain model must have a flexible structure to simulate the sequential production steps of electrode and cell production as well as flexible material flows in module and system assembly. As explained in Sect. 2.1.2, there are different types of material flow (e.g. diverging or converging) and production principles (e.g. job shop or line) of which the suitability depends on the product type. According to the product-process matrix presented by Hayes and Wheelwright (1979), job shop and disconnected line configurations are suitable for few unique product types with low volumes whereas continuous and connected line configurations are suitable for high volumes of standardized products. Flexible and agile production systems aim at handling high volumes of multiple product types (e.g. Langer and Altling 2000; Hu et al. 2011). An example of an agile process chain configuration is the matrix-structured configuration (Greschke and Herrmann 2014). Thus, the process chain model needs an adaptable modeling structure for imitating different process chain configurations and related control strategies. This is required to replicate existing systems as realistic as possible and to model innovative configurations and control strategies. Relevant for battery production are sequential assembly lines or job shops layouts as well as flexible configurations such as matrix-structured process chains. Due to their innovative character, matrix-structured process chains are not yet covered in established simulation tools for material flow analysis.

Matrix-structures avoid a constant cycle time and equip machines in a way that each can be used for the processing of different production steps of several product types (Greschke 2016; Greschke and Herrmann 2014; Schönemann et al. 2015). The redundancy of machine capabilities allows a flexible flow of processing units and results in a higher utilization of the process chain. This configuration is proposed for handling a high product variety with uncertain demands for each product type. Hence, it may be a feasible configuration for module and system assembly.⁶ Figure 4.8

⁶In general, the feasibility of a matrix-structure configuration strongly depends on the specific product types which should be produced or assembled. The realization of a flexible routing may be difficult for large and heavy products and limited due to space restrictions. Further information about the concept of matrix-structured production systems and its application and evaluation is

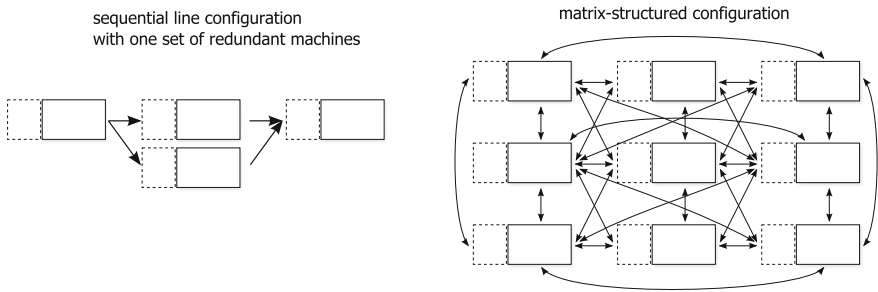


Fig. 4.8 Comparison of a sequential line with a matrix-structured configuration and the possible material flows

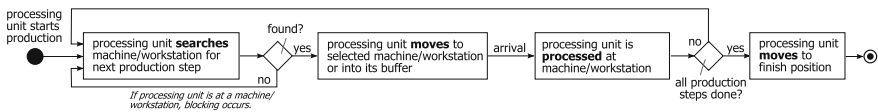


Fig. 4.9 Simplified logic of processing unit flow

illustrates the comparison of a sequential line configuration with a matrix-structured configuration indicating the possible material flows.

In order to achieve the required adaptable and flexible modeling of different process chain configurations and control strategies, the routing of specific processing units is based on autonomous decisions of processing units regarding selecting the next machine instead of being predetermined in the model configuration. Whereas traditional DE process chain models typically connect machines or processes corresponding to static directional material flows, the proposed model treats machines and the flow of processing units independently. This can be realized by a hybrid DE and AB simulation approach in which machines and processing units are modeled as individual agents. Machines offer capabilities for the processing of production steps and processing units select suitable machines for each production step. This logic enables to model any kind of process chain configuration and control strategy. Figure 4.9 illustrates the logic of the processing unit flow. Once a processing unit enters a process chain, it searches a suitable machine for the next production step. If one is found, the processing unit moves to the selected machine or its buffer. The processing starts after arrival or after the previous processing unit is finished. After completion of the production step, the processing unit searches a machine for the next production step or – if all production steps are completed – moves to the finish area. If no machine can be found and the processing unit is currently at a machine, the product unit cannot travel anywhere. In this case, the current machine is blocked until the product unit finds a next machine.

(Footnote 6 continued)
 published for example in Greschke (2016), Greschke et al. (2014), Greschke and Herrmann (2014), and Schönemann et al. (2015).

Control strategies contain rules and criteria for the selection of suitable machines and have to consider the given process chain configuration. Examples of control strategies are “shortest distance” or “shortest throughput time” (Schönemann et al. 2015).

Shortest distance The control strategy shortest distance aims at reducing the distance a processing unit has to travel through the process chain. After completion of a production step, a processing unit searches the next suitable machine based on the distance between the current location and the next machine. This strategy does not consider the overall lead time of a processing unit. This strategy might be favorable if the costs of transportation are high.

Shortest throughput time The strategy shortest throughput time aims at short waiting times for each processing unit resulting in short overall throughput times and a high system utilization due to reduced idling times of machines. A processing unit selects a machine which offers the processing of the next production step in the shortest period of time. According to this strategy, first all machines are checked whether they can process the next production step. Next, all suitable ones are analyzed regarding the time until each station could start processing. This time depends on the state of a machine (e.g. idle or processing), the amount of other products in the buffer, and on other processing units having reserved the machine.⁷ The strategy also considers the distance and velocity of the movement between the current location and the respective machine. The times until processing of all suitable machines are compared and the one with the shortest time until processing is selected.

Control algorithms based on these strategies require knowledge about the states and conditions of all machines. A processing unit has to know which machine is capable of processing the next production step, if a suitable machine is available (turned on, free, and not disturbed) or what the ramp-up time is, what the capacity or the current buffer level is, or how much remaining time it takes until the currently processed processing unit is completed. These dynamic properties are determined in models for each machine and provided as an input to the process chain model.

② → **Input:** properties and states of all machines from machine models.

In the other direction, the process chain model interacts with machine models by sending information about machine selection and arrival of processing units to models of machines which have been selected by a processing unit. This allows modeling the machine operations based on the dynamic scheduling and routing of jobs and related processing units.

⁷If a machine is currently in idle state and not reserved by other products, the time till processing is only determined by the movement. If a machine is currently processing another product, the remaining processing time as well as the processing times of products in the buffer has to be considered. If a machine is reserved by another processing unit, the time until processing is at least the time until the prior processing unit is finished.

Output → ②: information of processing unit flow and machine selection of processing units to machine models.

Control strategies have to consider different shift schedules. Often, facilities operate in two or three shifts per day each with defined working hours and break times. The process chain model has to define the working hours and rules about what happens with machines during non-working hours.

The described concept for process chain configuration and control strategies allows to model various kinds of process chains and material flows and to dynamically create schedules for machine operation which also influences the operation of TBS and workers.

4.3.3 State Variables and Indicators

Performance indicators are used to quantify the operation of a process chain and the surrounding infrastructure. They indicate the impacts of improvement measures and enable the comparison of different process chain configurations. The suggested indicators for this model are grouped into the categories energy flows, material inputs, costs of machine operation, as well as system utilization and processing unit flow.

4.3.3.1 Energy Flows

The total energy demand is relevant for the energetic evaluation of a process chain as well as for determining the embodied energy of individual processing units and the average of the embodied energy. Thus, one purpose of the process chain model is aggregating energy demands related to the operation of machines and to allocate these demands to processing units.

Energy Demand of Process Chain

The total power demand (in kW) of a process chain and its infrastructure over time PD_{TOTAL} is the sum of the aggregated power demands of all machines (PD_{MACH}) and the indirect power demand of the related TBS (PD_{TBS}).

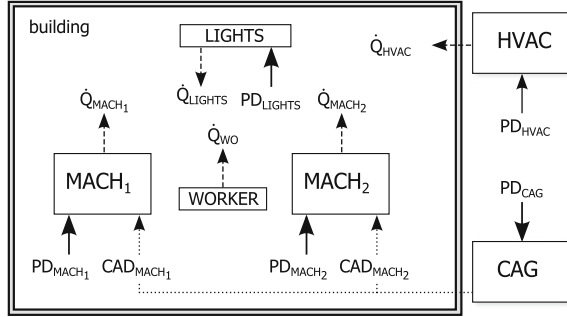
$$PD_{TOTAL}(t) = PD_{MACH}(t) + PD_{TBS}(t) \quad (4.1)$$

Figure 4.10 illustrates the considered energy flows related to machines and TBS for an exemplary building zone.

PD_{MACH} at time t is determined by summing up the power demands of all machines.

$$PD_{MACH}(t) = \sum_{mn=1}^{MN} PD_{MACH_{mn}}(t) \quad (4.2)$$

Fig. 4.10 Energy flows (PD: power demand, \dot{Q} : heat flow, CAD: compressed air demand, CAG: compressed air generation) for an exemplary building



Since machines and other equipment demand energy not only during processing but also during non-productive times (Gutowski et al. 2006; Devoldere et al. 2007), it is important to consider the actual power demand over time instead of the average power demand. The power demands of machines must be provided by machine models.

② → **Input:** power demand $PD_{MACH_{mn}}$ from machine models.

PD_{TBS} is determined by summing up the power demands of TBS systems. For battery production, relevant TBS are lighting, compressed air generation (CAG), and HVAC of all building zones.

$$PD_{TBS}(t) = PD_{LIGHTS}(t) + PD_{CAG}(CAD_{MACH}, t) + PD_{HVAC}(\dot{Q}_{TOTAL}, t) \quad (4.3)$$

The first term refers to the power demand of lights which is determined by a lighting model considering the required lighting intensity and efficiency for all building zones.

⑤ → **Input:** power demand PD_{LIGHTS} from lighting model.

Both the power demand of CAG and HVAC depend on different operational factors. PD_{CAG} depends on the compressed air demand CAD_{MACH} (in m^3/h) which is calculated by summing up the demands of all machines.

$$CAD_{MACH}(t) = \sum_{mn=1}^{MN} CAD_{MACH_{mn}}(t) \quad (4.4)$$

This demand is forwarded to the CAG model for determining PD_{CAG} .

② → **Input:** compressed air demand $CAD_{MACH_{mn}}$ from machine models.

Output → ④: total demand CAD_{MACH} to CAG model.

The CAG model has to return the determined power demand (e.g. for compressors) which is caused by the operation required to provide the requested amount of compressed air. The CAG model further determines the pressure within the CAG system which is a relevant information for machines (if the pressure is too low, a machine may not be able to operate).

- 5 → **Input:** power demand PD_{CAG} from the CAG model.
- 5 → **Input:** system pressure cap from the CAG model.

PD_{HVAC} depend – among other factors – on heat emissions \dot{Q}_{TOTAL} to the building. That means that the process chain model has to aggregate the heat emissions from various sources and forward this information for determining the power demands for heating, cooling, and ventilation. Machines demand power which is transformed into heat and emitted to the building (\dot{Q}_{MACH}).

- 2 → **Input:** heat emissions $\dot{Q}_{MACH_{mm}}$ from machine models.

Furthermore, lights are heat sources emitting heat (\dot{Q}_{LIGHTS}) depending on the schedule (Ryckaert et al. 2010) and type of light source.

- Output** → 5: signals for turning lights on and off to the lighting model.
- 5 → **Input:** heat emissions \dot{Q}_{LIGHTS} from lighting model.

In addition, workers emit heat depending on their activity level (Harriman 2002). The behavior of workers, depending on required machine operation and schedules, can be modeled in more detail consider different levels of activity.

- Output** → 4: required activity of workers to worker models.
- 5 → **Input:** heat emissions of workers \dot{Q}_{WO} from worker models.

In general, heat can also be emitted by products (here: processing units) if their temperature is increased during processing (Wright et al. 2013). However, this is usually not relevant in battery production. Consequently, the total heat emissions can be calculated by summing up all heat emissions.

$$\dot{Q}_{TOTAL} = \dot{Q}_{MACH} + \dot{Q}_{LIGHTS} + \dot{Q}_{WO} \tag{4.5}$$

These heat emissions act as heat gains inside the building and may cause a temperature increase. Thus, the process chain model has to communicate the heat emissions to the building model which determines the resulting inside temperatures.

Output → **6**: total heat emissions \dot{Q}_{TOTAL} to building model.

The building model provides the indoor temperature to the HVAC model which calculates the required heating or cooling loads and the resulting power demand.

5 → **Input**: power demand of HVAC system PD_{HVAC} from HVAC model.

Besides electricity, HVAC systems often use gas or district heat for heating or dehumidification. These demands can also be collected within the process chain model.

Since the requirements regarding indoor environment (e.g. temperature, humidity, cleanness, illumination) are not necessarily the same for an entire building, it is proposed to define building zones with identical conditions.⁸ Hence, heat emissions have to be allocated to building zones. This requires knowledge about the location of heat sources within the building. Machines can be allocated to zones based a process chain layout and lights can directly be associated to a zone. Workers, however, can move inside the building and across building zones. Worker models must be able to simulate the movement and location of all workers within the building.⁹

4 → **Input**: current locations of workers from worker models.

The total power demand is base for the calculation of the total energy demand ED_{TOTAL} during a period of time (t_{start} until t_{finish}).

$$ED_{TOTAL} = \int_{t_{start}}^{t_{finish}} PD_{TOTAL}(t) dt \quad (4.6)$$

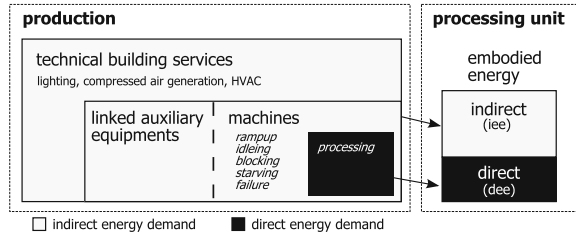
This total energy demand can be further broken down into the used energy carriers. While machines, lighting, and compressed air generation usually require electric energy, energy for building heating is often generated from natural gas or provided as district heat. This breakdown of energy carriers as well as the related consumption pattern is important since different energy carriers may cause different energy costs (depending on the specific energy supply contract). As an example, industrial supply contracts for electricity often determine the costs considering the electrical peak power demand in addition to the total energy demand (Thiede et al. 2013b). Moreover, the environmental impacts related to energy use differ for each energy carrier. For example, the equivalent CO₂ emissions per generated kWh depend on the regional electricity mix.¹⁰

⁸The differentiation of building zones is common for building simulation and also suggested by Seow and Rahimifard (2011) for the allocation of indirect energy demands to specific processes.

⁹Tracking of heat flows from movable objects to the building is proposed by Wright et al. (2013).

¹⁰The equivalent CO₂ emissions from electricity generation in the German electricity mix in 2014 are 0.609 kg CO₂^{eq}/kWh (Umweltbundesamt 2015).

Fig. 4.11 Allocation of direct and indirect energy demands of production to direct and indirect shares of embodied energy per processing unit; Figure inspired by Posselt et al. (2014)



Embodied Energy of Processing Units

With reference to Seow and Rahimifard (2011), the embodied energy of products is another interesting indicator. In the process chain model, the embodied energy of a processing unit is made up of the direct and indirect energy demands which are allocated to this unit. Direct energy demands are related to the actual value adding activity. Indirect energy demands are caused by non-value adding activities as well as the services and infrastructure needed to maintain the required conditions for the processing. Figure 4.11 illustrates the allocation of energy demands to the direct and indirect shares of embodied energy.

In the model, the direct embodied energy dee_{pun} of a processing unit is determined by integrating the power demands of the utilized machines¹¹ over the processing times (from $t_{start,ps}$ to $t_{finish,ps}$) of all production steps ($ps = 1, \dots, nps_{pm}$) of the particular processing unit divided by the quantity of processing units qpu_{MACH} which is simultaneously processed in a machine.

$$dee_{pun} = \frac{\sum_{ps=1}^{nps_{pm}} \int_{t_{start,ps}}^{t_{finish,ps}} PD_{MACH} dt}{qpu_{MACH}} \quad (4.7)$$

There are different strategies for allocating indirect energy demands from machines in idle state or peripheral equipment and TBS to the indirect embodied energy iee_{pun} of processing units. The process chain model allows to evaluate the impacts of different allocation strategies. One strategy is to subtract the sum on the direct embodied energy demands of all processing units being finished during an observed period of time from the total energy demand and to divide the remainder by the quantity of finished processing units $qfpu$.

$$iee_{pun} = \frac{ED_{TOTAL} - \sum dee_{pun}}{qfpu} \quad (4.8)$$

It could also be the case, that compressed air is required for the actual processing of processing units. In this case, a share of the energy demand for compressed air

¹¹In this model, energy demands of linked auxiliary equipment and services directly related to a machine during the processing state are also considered as direct energy demands.

generation could be assigned to the direct embodied energy of the certain processing units. Moreover, if not all processing units are being processed inside all building zones, it is also possible within the model to allocate the energy demands of building zones (e.g. of a dry room) only to processing units which were processed inside these zones. The allocation of indirect energy demands was discussed in detail by Posselt et al. (2014).

The embodied energy of a processing unit indicates how much energy was used for the production. If a processing unit is used to create another processing unit (e.g. cells are assembled into a module), the embodied energy has to be added to the embodied energy of the receiving processing unit. A breakdown of the embodied energy allows determining energetic hot-spots as well as evaluating impacts of process parameters (on direct energy demand) and production strategies such as different batch or buffer sizes (on indirect energy demand).

4.3.3.2 Material Inputs

During processing, the transformation of a processing unit is carried out using energy and materials. For example, in the mixing process, diverse materials are fed into a mixer to create a viscous slurry. Since materials contribute to a large share of costs and environmental impacts of batteries, the evaluation of required materials is relevant. The process chain model can allocate consumed material fractions to processing units and determine the increase of material costs along the process chain. The model contains a set of material types MAT_{matn} (with number $matn = 1, \dots, MTN$) and related prices $MATP_{matn}$. During processing, an amount of a material type $mata_{matn}$ is added to the processing unit along with cost information. The material costs of a processing unit $matc_{pun}$ can be calculated during production by multiplying the embodied amount of each material type with the unit price.

$$matc_{pun} = \sum_{matn=1}^{MATN} mata_{matn} \cdot MATP_{matn} \quad (4.9)$$

The necessary amount of each material per production step $mata_{matn}^{PS_{pm,i}}$ can be defined for each process within the process chain model or within process models and provided to the process chain model.

3 → **Input:** amount of each material type $mata_{matn}^{PS_{pm,i}}$ for production step i of product type ptn from process models.

Beside direct material demands of processes, machines and processes often require indirect auxiliary materials such as lubricants or other media. These indirect material demands are determined within each machine and aggregated per auxiliary material type $AUXMAT_{auxmatn}$ on processes chain level. These demands can be allocated to processing units in the same manner as indirect energy demands.

2 → **Input:** amount of each auxiliary material type $auxmata_{auxmat,mm}$ of all machines from machine models.

In a similar way, environmental impacts related to the amount of used material can be added to processing units for each material type. The environmental impact of materials can be represented by equivalent CO₂ emissions (kg CO₂^{eq}/kg). This allows determining the current environmental impacts cause by finished and semi-finished processing units at a specific point in time.

4.3.3.3 Costs of Machine Operation

The operation of machines induces fix and variable costs. Examples of fix costs are costs resulting from depreciation, interests, insurances, used building space, etc. Examples of variable costs are costs due to maintenance and repairs, energy demand, auxiliaries (e.g. lubricants), etc. To assign the costs of machine operation to a processing unit, machine-hour rates can be derived from the sum of all costs related to the operation of a machine divided by the annual usage of the machine (Plinke and Rese 2006). The process chain model allows to allocate defined machine-hour rates MHR_{mm} for each machine (in EURO/h) to processing units depending on the time spent on a specific machine.

4.3.3.4 System Utilization and Processing Unit Flow

The utilization of a process chain and the flow of processing units are relevant indicators for the economic evaluation of process chains.

Utilization

The utilization of a process chain uti_{PC} or a machine uti_{MACH} is defined by the ratio of productive time shares and overall available production time. Figure 4.12 illustrates the operational time shares of a machine as fractions of the available production time (e.g. shift time). A machine is only productive in processing state and not if it is in idle state (e.g. during break times or if no jobs are available), blocked, or in failure state.

In the model, the utilization of a process chain at a specific point in time t $uti_{PC,t}$ is determined by the ratio between the quantity of machines processing and the total quantity of machines. For example, if four machines out of ten machines are processing at time t , $uti_{PC,t}$ is 40%. The mean utilization of a process chain $uti_{PC,mean}$

available production time (e.g. shift time)				
productive time share (processing)	breaks	machine failures	blocking	starving

Fig. 4.12 Operational time shares of a machine during the available production time

for an observed time period (e.g. shift or week) can be determined as the mean of uti_{PC} .

Yield

The yield Y_t^{pm} at time t is the output of finished processing units of type pm in the desired quality (reduced by the discarded units) during a time period from start of production until t. The yield refers to a job of a product type (e.g. yield of cells). This indicator is important for the allocation of indirect energy demands and production costs.

Production Lead Time of Jobs

The production lead time pl_{jn} of a job is the time between the introduction of the first processing unit of a job to the process chain ($t_{jobstart_{jn}}$) until the last processing unit is finished ($t_{jobfinish_{jn}}$). This time can be determined for each job but the average lead time apl_{pm} resulting from all jobs is also relevant for the evaluation of the overall performance of a process chain. This average is calculated by dividing the sum of the lead times by the yield.

Value Adding and Non-value Adding Time Shares

The ratio of value adding to non-value adding time shares describes how fluent processing units travel through the process chain. Figure 4.13 illustrates the different time shares of the lead time of a processing unit. This sequence corresponds to the processing unit flow logic shown in Fig. 4.9.

The only value adding activity is the processing in a machine. All other activities such as handling, movement, or waiting occur during production but do not directly add value. The value adding time share of a processing unit is determined by adding the processing times of all production steps. The value must be divided by the entire lead time of the processing unit. The ratio can also be calculated for jobs by considering the time shares of the associated processing units.

Blocking

Whenever a processing unit cannot leave a machine because no next machine is available, the current machine gets blocked. No new processing unit can enter the machine because the finished processing unit is still present. Such blocking causes waiting times for processing units and idle times for blocked machines and consequently result in non-value adding time shares and energy demands. The process chain model can determine the quantity of occurring blocking and the related production steps which caused each blocking. This enables the identification of bottlenecks.

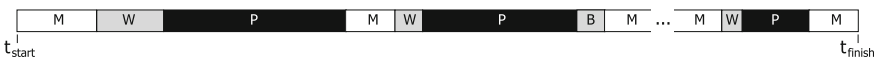


Fig. 4.13 Time shares of processing unit flow during production (M: moving; W: waiting; B: blocked; P: processing)

All described performance indicators can be used for evaluating different aspects of the process chain operation which is effected by the behavior of its various elements and the surrounding infrastructure. The consideration of relevant cause-effect relationships between model elements requires detailed modeling.

4.4 Concepts for Sub-models

The different models presented in the framework have to be further defined regarding the required inputs, the inherent model logic, and the output results. First, a model concept is proposed for machine models (Sect. 4.4.1). Second, a concept for modeling product characteristics and specifications is explained which can be combined with process models describing the creation and transformation of product characteristics (Sect. 4.4.2). Third, a concept for human worker activity modeling is presented (Sect. 4.4.3). Fourth, concepts and relevant aspects are derived for modeling of the operation of TBS systems (Sect. 4.4.4) for lighting, compressed air generation, and HVAC. Fifth, it is explained how a building model can describe the interactions of a building with the surrounding environment and how the inside conditions can be determined in order to derive required heating and cooling loads (Sect. 4.4.5).

4.4.1 *Machine Models (2)*

The behavior and operation of each machine within the process chain needs to be described by a machine model. The purposes of machine models are

- modeling of machine operation over time according to the schedule provided by the process chain model,
- description of machine states of entire machines or for all relevant components,
- determination of demand profiles for energy carriers and resulting heat emissions, as well as
- modeling the machine failure behavior.

Machine models can be developed and configured based on production data and measurements (e.g. Herrmann et al. 2011) or by using mathematical equations describing the machine operation based on physical effects (e.g. Eisele 2014; Heinzl et al. 2012). Furthermore, machine models can be of different detail (Hesselbach 2012). On the one hand, a machine can be treated as a black box. On the other hand, machines can be described in more detail by modeling the operation of each component. As a minimum requirement for the multiscale simulation, machine models have to describe machine states, the transition conditions between states, and parameters associated to states (e.g. energy demand during idle). Moreover, the compressed air demand and heat emissions of a machine have to be calculated. Information about states,

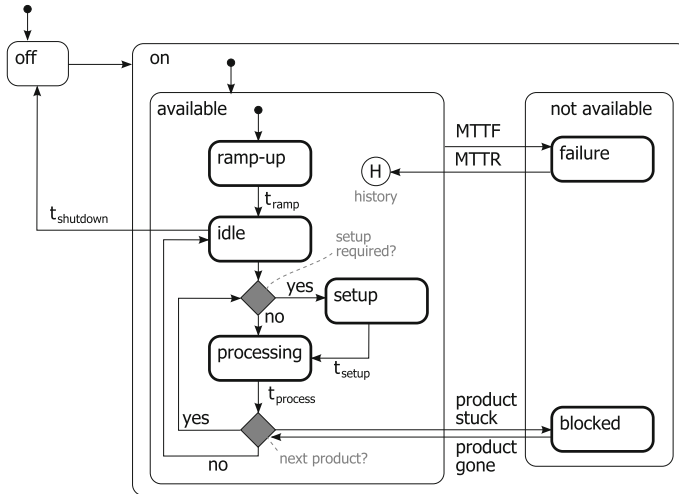


Fig. 4.14 Generic state chart for modeling of the machine operation

demands, and emissions is required by the process chain model. To fulfill the minimum requirements, a generic state-based machine model – applicable for any kind of machine type – can be parametrized for specific machines.

4.4.1.1 Generic Machine Model

Machines can be described by static properties such as geometrical dimensions, capacity and buffer size, as well as by dynamic characteristics such as electric power and compressed air demands, media demands (e.g. cooling lubricant), and heat emissions. The dynamic characteristics depend on the machine state.

Machine States

During production, a machine can be in different operational states with specific transition conditions between these states. All machines can be described by generic states such as off, on, ramp-up, idle, setup, processing, blocked, and failure. Thus, a generic state chart has been created to model the behavior of a machine in a generic manner (similar as in Schönemann et al. 2015; Mousavi et al. 2015; Thiede 2012; Dietmair et al. 2009). This chart is shown in Fig. 4.14. Initially, a machine is in off state and it is turned on if the model receives the signal from the process chain model, that it has been selected by a processing unit.

1 → **Input:** signal about allocation of processing unit to machine from process chain model.

When a machine is turned on, it is in the ramp-up state until it switches to idle state after the ramp-up time t_{ramp} . When a processing unit arrives, the machine switches into processing or setup state.

1 → **Input:** signal about arrival of a processing unit (and its product type) from process chain model.

If the product type requires a setup, the machine switches to processing state after the setup time t_{setup} . After the processing time $t_{process}$, the processing unit will leave the machine. If the processing unit has left and a next processing unit is waiting for processing, the machine will switch to setup or processing state again. If no further product is available for processing, the machine switches to idle state. If no next processing unit arrives for processing, the machine is switched off after the shutdown time $t_{shutdown}$. If a processing unit cannot leave the machine after processing (if no next machine is available), the current machine switches to the blocked state and stays in this state until the processing unit leaves.

1 → **Input:** signal about leaving of processing unit from process chain model.

If a machine failure occurs, the machine switches from the available to the failure state. Processing units which are currently processed stay in the machine until the failure is repaired. The time between failures is represented by the MTTF. The time until a failure is resolved is represented by the mean time to repair (MTTR). These times are usually modeled by using probability distributions which describe the characteristics of each machine.¹² The history element (H) indicates that when a failure is resolved, the state chart switches to the state within the available state in which the failure occurred.¹³ Information about each state change is provided to the process chain model.

Output → **1**: states and conditions of machine to process chain models.

¹²In general, any kind of probability distribution can be used for describing MTTF and MTTR. However, often a Weibull function is used since it is flexible and can be configured by defining suitable scale and shape parameters (Birolini 2010).

¹³This assumption is not always valid. It is possible that failures required a machine to be switched off completely or that the currently processes product units will not be further processed.

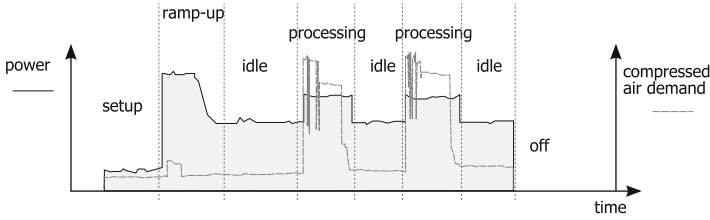


Fig. 4.15 Exemplary power load profile of a machine with associated operational states

Electric Power and Compressed Air Demands

The process chain model requires information about the machine's power demand $PD_{MACH_{mn}}$ and compressed air demand $CAD_{MACH_{mn}}$. Both the power and compressed air demands depend on machine states. Figure 4.15 illustrates an exemplary power demand profile of a machine for different states. In the generic model, the power demand of a machine is modeled by an average power demand value for each state, i.e. one (electric) power demand value $PD_{MACH_{mn}^{state}}$ and compressed air demand value $CAD_{MACH_{mn}^{state}}$ for each state. These values can be determined by measurements or estimated based on manufacturers specification and the nominal power of a machine. The power demand profile can show different profiles depending on the type of machine.

Output → ①: power demand $PD_{MACH_{mn}}$ to process chain model.

Output → ①: compressed air demand $CAD_{MACH_{mn}}$ to process chain model.

Heat Emissions from Machines

During the operation of a machine, the supplied energy is partially converted into heat due to conversion losses and inefficiencies.¹⁴ These internal heat sources lead to a continuous increase of the machine temperature until a steady state is reached. The warm machine emits heat $\dot{Q}_{MACH_{mn}}$ from the machine surface to the building environment through convection and radiation¹⁵ (Hesselbach 2012). The thermal behavior of a machine has to be modeled with a different approach compared to power and compressed air demand since the system reacts slower on changes induced by different states. The machine slowly heats up after it is turned on and it cools down after it is turned off. The heat transfer through convection can be calculated base on the convective heat transfer factor α , the machine surface area A_{mn} and the temperature difference between the machine temperature at the surface T_{mn} and the air temperature of the building zone T_z (Lampinen et al. 2007).

$$\dot{Q}_{conv} = \alpha \cdot A_{mn} \cdot (T_{mn} - T_z) \quad (4.10)$$

¹⁴A comprehensive description of energy conversion in factories can be found in Posselt (2016).

¹⁵Heat transfer through conduction can be neglected since air has a low thermal conductivity.

The heat transfer through radiation can be determined based on the emissivity¹⁶ of the machine ε_{mn} , the Stefan-Boltzmann constant¹⁷ σ , the machine surface area A_{mn} and the temperature difference between T_{mn} and T_z to the fourth power.¹⁸

$$\dot{Q}_{rad} = \varepsilon \cdot \sigma \cdot A_{mn} \cdot (T_{mn}^4 - T_z^4) \quad (4.11)$$

6 → **Input:** temperature of building zone T_z from building model.

The thermal behavior of a machine can be modeled at different levels of detail. In the generic machine model, a machine is considered as a mass (of one material) which is sufficient for a first analysis of the thermal behavior. For simplification, heat emissions from the machine through radiation are neglected. This allows calculating the machine temperature with the following equation¹⁹ (Hesselbach 2012).

$$\dot{T}_{mn} + \frac{\alpha \cdot A_{mn}}{m_{mn} \cdot c_{mn}} \cdot T_{mn} = \frac{\dot{Q}_{HS_{mn}} + \alpha \cdot A_{mn} \cdot T_z}{m_{mn} \cdot c_{mn}} \quad (4.12)$$

The heat source \dot{Q}_{HS} is simplified modeled as the electrical power input to the machine reduced by an efficiency factor η indicating the share of power which is not converted into heat (e.g. converted into internal energy).

$$\dot{Q}_{HS_{mn}} = PD_{MACH_{mn}}(t) \cdot (1 - \eta) \quad (4.13)$$

The described equations can be used to determine the total heat emission of a machine $\dot{Q}_{MACH_{mn}}$. This value is passed to the process chain model for the calculation of the entire internal heat gains of a building zone.

Output → **1**: heat emissions $\dot{Q}_{MACH_{mn}}$ to process chain model.

In summary, the generic machine model enables the simulation of sequences of machine states based on commands from the process chain about the production program. It enables the generation of state-based profiles for power demand, compressed air demand, and heat emissions. However, the generic models considers a machine as a black box and relies on various assumptions. Consequently, the accuracy of the

¹⁶Emissivity values of polished aluminum and polished steel are 0.77 or 0.15, respectively.

¹⁷ $\sigma = 5.6703 \cdot 10^{-8} \text{ W/m}^2\text{K}^4$.

¹⁸Heat exchange through radiation occurs between the machine surface and the surrounding surfaces such as walls, the ceiling, or other machine surfaces. For simplification, Hesselbach suggests to use the average room temperature to determine the temperature difference (Hesselbach 2012).

¹⁹The equation is derived from the law $Q = m \cdot c \cdot \Delta T$ which defines the heat required to increase the temperature of a body by ΔT . The acting heat flows are the internal heat source reduced by heat emissions to the building environment. This leads to $m \cdot c \frac{dT_m}{dt} = \dot{Q}_{HS} - \dot{Q}_{con} - \dot{Q}_{rad}$. For simplification, radiation is neglected in Eq. 4.12.

achievable results is reduced in favor of modeling complexity. If a higher accuracy is required, machine models can be of more detail in different regards.

4.4.1.2 Detailed Machine Model

Detailed models can substitute a generic machine model or be used in addition to determine the previously defined model outputs based on the defined inputs. This may become relevant since many modern machines can contain several functions such as performing different processes, tool change, waste removal, and others (Gutowski et al. 2009). Thus, the states of a machine can be broken down further compared to the generic model. Hence, a generic model may not provide the necessary functionality to imitate the machine behavior correctly. In this case, detailed models can describe physical effects within the machine as well as the behavior and interactions of different machine components. Depending on the components of a machine, on a lower level, more specific states can be differentiated for individual machines. As examples, a mixer could have the states “low intensity mixing” and “high intensity mixing” and component specific transition conditions.

Power and Compressed Air Demand

The power demand of a machine is the sum of the power demands of all components (e.g. Dietmair et al. 2009).

$$PD_{MACH_{mn}}(t) = \sum_{c=1}^C PD_{mn_c}(t) \quad (4.14)$$

C indicates the number of different components. Likewise, the compressed air demands is the sum of the demands of all components (e.g. grippers).

$$CAD_{MACH_{mn}}(t) = \sum_{c=1}^C CAD_{mn_c}(t) \quad (4.15)$$

The power demands of each component can be either determined by measurements or by physical modeling such as presented in Eisele (2014) and Schrems (2014). Abele et al. presented a combined approach of machine and process modeling for determination of a machine’s power demand (Abele et al. 2015). In every case, the operational states of components have to be linked to the overall states of the machine. The advantage of component based models is the possibility to identify components with high energy demands. These components can be modeled with greater detail to improve the machine model accuracy. Moreover, the effect of shutdown strategies or stand-by modes can be tested for these components within simulation experiments. Furthermore, the power demand of the entire machine within the different generic states can be modeled at higher resolution since components can switch between their states within the superordinate processing state.

Heat Emissions

Instead of treating a machine as one mass with one internal heat source, the thermal modeling of a machine can be detailed by dividing a machine in different virtual layers or by considering multiple internal heat sources induce by different components as well as additional heat flows out of the machine (e.g. through cooling systems or products) (Hesselbach 2012). A layered model allows imitating the heat distribution inside a machine and a more accurate calculation of heat emissions. Moreover, this enables predicting the thermal conditions within a machine. Knowledge about these conditions may be relevant for processes which rely on constant or specific temperatures (e.g. a furnace with a temperature profile).

Failure Behavior

Machine models on component level allow modeling the failure behavior of components. This may be more accurate compared to a black box machine model and could be relevant for analyzing maintenance strategies. Detailed models can be used to specify MTTF and MTTR for each component. In addition, the consequences of the failing of a particular component can be specified within the model logic. Some failures allow further machine operation but result in decreased product quality while other failures impede further use of the machine until completed repair.

As disadvantages, detailed models are more complicated to develop, have higher requirements regarding computational power, and need longer to compute. Furthermore, in general they rely on assumptions due to missing detailed information and data about machines properties such as component behavior, materials, heat transfer coefficients, etc. Thus, the trade-off between potentially higher accuracy – of detailed models compared to the generic model – and higher modeling effort has to be evaluated carefully. In some cases, combinations of generic machine models with detailed specific models for certain aspects may provide better simulation results and foster a deeper system understanding without causing very high modeling effort. Figure 4.16 presents the advantages and disadvantages of both generic and detailed machine models.

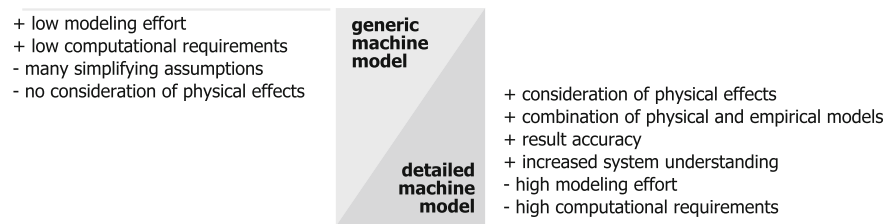


Fig. 4.16 Advantages and disadvantages of generic and detailed machine models

4.4.2 Product and Process Models (3)

On the one hand, various factors during cell production and system assembly influence the performance and quality of final cells and battery systems. On the other hand, product specifications of cells and systems influence the operation of machines and process chains, affecting also other production system element. Simulating these influences requires models for describing the specifications and characteristics of processing units during production as well as models for processes describing the creation and modification of product characteristics.

4.4.2.1 Product Model

In the multiscale simulation, product models characterize processing units during production regarding their specifications and current characteristics. The purposes of product models are

- providing information about the required production steps, processes, usable machines, and related product specifications,
- describing the evolution of product characteristics along all production steps, and
- tracking and storing information about the production progress.

A product model has to relate to one particular processing unit which is associated to a subordinate job. A processing units track the existing and created product characteristics as well as time stamps for each production step. The defined job structure of associated processing units allows to exchange product characteristics between different processing units within one job. This is important if processing units become parts of other processing units and the characteristics of the latter depend on the characteristics of the former. An example is the assembly of multiple electrodes with specific characteristics into cells.

Output → ③: product specifications to process models.

③ **Input** → : product characteristics from process models.

In order to describe the characteristics of a processing unit during production, a set of characteristics $PCHAR_{pm}$ can be defined for each product type. These characteristics can be created or transformed within processes. Wuest (2015) developed a concept for describing and tracking of product characteristics along a process chain enabling examining the effects of created or transformed characteristics on consecutive processes. Following this concept, semi-finished processing units can be in different states during production where state 0 is the state prior to production (raw materials) and state nps_{pm} is the final state after completing the last production step. Figure 4.17 illustrates the concept of product states and the related product characteristics (A, B, ...). The figure shows that product characteristics can be created (indicated by *) or transformed (indicated by ') from one product state to another.

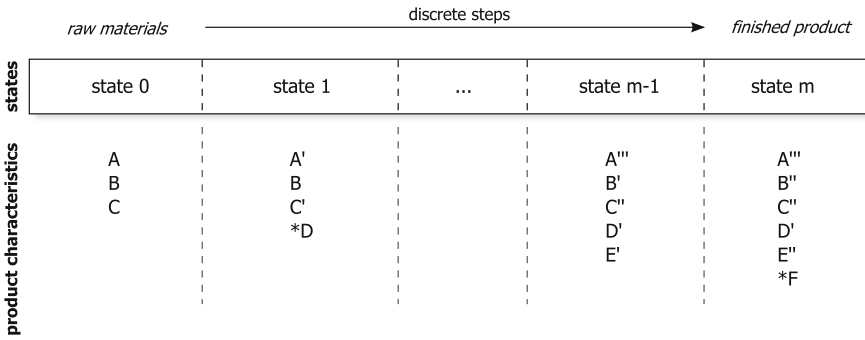


Fig. 4.17 Generic states ($0-nps_{pm}$) and exemplary characteristics (A–F)

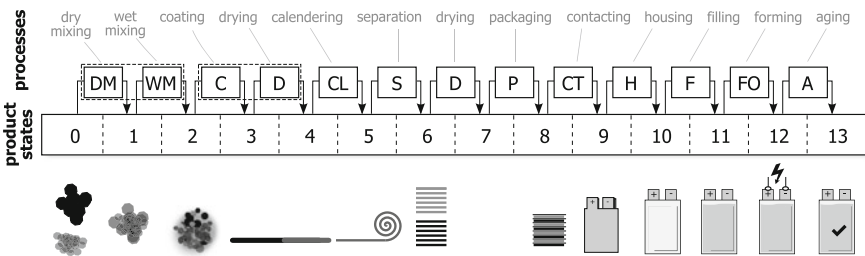


Fig. 4.18 Process chain and product states in cell production

The transition from one state to another is realized with processes. This product model concept can be applied to any product type. The model development requires the identification of all product states during production and the related product characteristics. Following the defined system boundaries, product models have to be differentiated for electrodes and cells as well as for modules and systems.

Electrodes and Cells

In general, the production of (LIB) cells requires 13 different processes (see Sect. 2.1.3) whereas the first seven processes of electrode production are the same for both anodes and cathodes. Consequently, there are 14 different product states within cell production whereas states 1–7 are differentiated for anodes (a) and cathodes (c). In these first seven states, anodes and cathodes have the same characteristics but each of them potentially with different values. Figure 4.18 illustrates the product states of anodes, cathodes and cells during production with the related processes.²⁰

Product state 0 in the product model refers to the raw materials and their specific properties (e.g. size, shape, and morphology of particles). State 1 refers to the prepared materials with the characteristics weight fraction of each added material,

²⁰Here, separation is considered as one process although in reality it could be differentiated between slitting of coils to width and cutting of individual electrode sheets.

conductivity, and packing density. State 2 refers to the finished slurry with the characteristics weight fractions, homogeneity, solid content, surface tension, viscosity, and slurry density. The created slurry is coated on the collector foil and immobilized by the drying process. State 3 refers to the foil with wet coating layer and state 4 refers to the dried electrode coil. The coating procedure has substantial influence on the homogeneity and thickness of the coating layer. Furthermore, relevant characteristics of state 3 are the coating length l_c and width w_c as well as the realized mass load m_L , the coating layer density and the wet coating thickness. Moreover, relevant are the properties of the collector foil (e.g. material, density, thickness). The drying process influences the distribution of the binder which is dissolved in the coating layer, the evaporation of the solvent, the adhesion of particles to the collector foil, as well as the porosity of the dried coating layer (state 4). The coated electrode is compressed in the following calendaring process. State 6 refers to the compressed electrode. The calendaring process has influence on the density of the coating, coating layer thickness, electrode thickness and porosity, pore radius, as well as the adhesion to the current collector (Haselrieder et al. 2013). State 6 refers to the separated electrode unit which will be processed in the later cell assembly. The main characteristics of state 6 are cutting quality (e.g. form tolerance, cutting edge clearness), and loose particle accumulations²¹ (Baumeister and Fleischer 2014). State 7 refers to the dried electrodes. State 8 refers to the created package. Characteristics are the number of anodes and cathodes, the accuracy of the electrode positioning, as well as the balancing of the electrode capacities (Schmitt et al. 2014). Also the separator is added which can be specified by its material properties. In the following processes, the arrester are connected to the current collector (state 9), the package is housed (state 10) and the housing is filled with electrolyte (state 11). Relevant characteristics of these states are the quality of the contacting weld (state 9), the amount of electrolyte and the wetting distribution inside the cell (state 11). The last processes after the assembly are forming and aging. During formation, a cell is initially charged which activates the active material. A low current is used to form the SEI layer on anodes (Yoshio et al. 2009). Measurements are taken for the cells open circuit voltage (OCV) and capacity (state 12). After forming, the cells are stored (aging) at a defined SOC (state 13). Table 4.1 lists the states of electrodes and cells with related processes as well as created and transformed product characteristic.

A job refers to the production of a quantity of cells. It triggers the production of anodes and cathodes as well as the assembly of cells. The electrode coils are produced in a sequence of batch processes. The coils are separated into single electrode sheets. Consequently, the product states of the electrodes have to be differentiated for anodes and cathodes and allocated to each single electrode sheet. The cells are assembled in unit processes. Consequently, each cell has its own states and values of characteristics. The characteristics of electrodes have to be forwarded to each processing unit representing a cell. These relations are shown in Fig. 4.19.

²¹ As explained, there may also be a differentiation between slitting of electrode coils and the cutting of single electrode sheets. Thus, there may be another state in the product model.

Table 4.1 Product states, characteristics, and related processes for cell production

State	Description	Previous process	Created characteristics	Transformed characteristics
0	Raw material: active materials, additives		Raw material properties; particle size(s); density(ies); CB agglomerate size	
1 _{a/c}	Mixed material fractions	Dry mixing	Weight fractions; conductivity; packing density	
2 _{a/c}	Slurry	Wet mixing	Coatable amount; viscosity; solid content; homogeneity; surface tension	CB agglomerate size; weight fractions
3 _{a/c}	Coated foil	Coating	Homogeneity of layer; mass load; wet coating thickness; collector properties	
4 _{a/c}	Dried electrode	Drying	Electrode thickness; remaining solvent content; binder distribution; particle adhesion; porosity; density	Pore diameter
5 _{a/c}	Compressed electrode	Calendering		Electrode thickness; coating thickness; density of coating; particle adhesion
6 _{a/c}	Separated electrodes	Slitting, cutting	Electrode geometry, cutting quality; particle accumulations	
7 _{a/c}	Dried electrodes	Drying	Remaining water content	
8	Wrapped electrode stack/winding	Folding, stacking, winding	No. of layers; placement accuracy; capacity; separator porosity; separator thickness	
9	Contacted electrode package	Contacting	Quality of arrester welds	
10	Pouch package	Housing	Housing material	
11	Assembled cell with electrolyte	Filling, closing	Amount of electrolyte; wetting distribution	
12	Formed and activated cell	Forming	SOC; OCV; SEI	
13	Finished cell	Aging	Storage duration	SOC

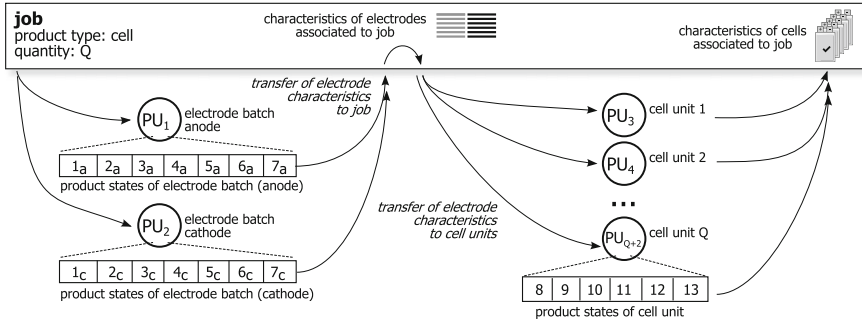


Fig. 4.19 Schema for the transfer of product characteristics between processing units and the subordinate job (exemplary for a job of cells)

Modules and Systems

Battery modules and systems can also be described during assembly by states with related processes characteristics. Product state 0 refers to the cells and components required for the assembly of a module. In the first process, cells are inspected. It is essential to combine cells within a module which have the same performance. The combination of cells with different performance may have negative impact on the entire module whose behavior is determined by the weakest cell. Similar to the selective assembly of electrodes into cells (Schmitt et al. 2014), strategies and measures for selective and adaptive assembly may be reasonable for module assembly. State 1 refers to the tested selected cells. State 2 refers to the pre-assembled cells and state 3 refers to the contacted cells. A relevant characteristic in state 3 is the quality of the welds which is checked by a voltage test. State 4 refers to a module with installed circuit board and sensors. State 5 refers to the entire assembly after testing. The module is in state 6 after the mounting of cooling plates and in state 7 after housing. State 8 refers to a tested finished module.

State 9 describes the assembly of modules on a base plate and state 10 refers to the final housed assembly. After the initial charging, a system is in state 11. A completed system after testing is in state 12. The states of a module and a system with the related processes as well as created and transformed characteristics are listed in Table 4.2.

A job may refer to the assembly of a quantity of modules or systems. In module assembly, the characteristics of selected cells must be copied to the characteristics of the containing module. In system assembly, the characteristics of cells contained in modules have to become part of the system’s characteristics.

In summary, the derived product model can describe the states of processing units during production and the related characteristics. Specific product models can contain parameters for defined product specification as well as variables and arrays to represent product characteristics for each processing unit.

The presented product states and related characteristics cover the characteristics which are often discussed in literature. However, the proposed product model allows to easily extend the set of modeled characteristics to represent specific LIB sys-

Table 4.2 Product states, characteristics and related processes for module and system assembly

State	Description	Previous process	Created characteristics	Transformed characteristics
0	Cells and components		Cell types	
1	Selected cells for module assembly	Inspection	Characteristics of cells	
2	Assembled cells	Pre-assembly	Number of cells per assembly; capacity; voltage; current	
3	Assembled and contacted cells	Contacting	Quality of joints; internal resistance	
4	Assembly with circuit boards and sensors	Installation of circuit boards and sensors	Number of sensors	
5	Tested assembly	Testing	State of assembly	
6	Assembly with cooling system	Cooling plate installation		
7	Housed module	Housing		
8	Tested module	Testing	State of housed assembly	
9	Modules on system base plate	Module placing and fixation	Capacity; voltage; current	
10	Housed components	Component installation and housing		
11	Charged and flashed (software) system	Flashing and charging	SOC	
12	Closed housing which is tested regarding leak-tightness	Closing and testing		

tems or other battery types. The exact creation and transformation of the product characteristics can be defined within process models.

4.4.2.2 Process Models

The purpose of process models is determining resulting product and process characteristics for each product state (of a processing unit) considering the influences between product specifications, process parameters, existing product characteristics, and various other direct and indirect internal and external factors (e.g. Winter 2016). Product characteristics can be created or transformed during processing of a production step. In a deterministic case, process models determine values of product

characteristics – based on relationships between specification and process parameters – and store this information within a product model of a particular processing unit. The resulting values of product characteristics can be predefined in a process model (e.g. based on experimental results or desired values) or calculated based on mathematical equations.

3 → **Input**: product specifications from product model.
Output → **3**: product characteristics to product model.

However, the results of production processes are subject to variations and accepted within defined tolerance limits (Geiger and Kotte 2005; Brüggemann and Bremer 2015). The variation of processing results can have different origins. Variation can be induced by machines (e.g. through geometric or thermal errors), process parameters (e.g. inaccurate setting of velocities or temperature profiles), materials (e.g. insufficient quality or wrong amounts), method or process selection, environmental conditions (e.g. temperature or humidity), as well as by humans being involved in the process²² (Wuest 2015; Brüggemann and Bremer 2015).

2 → **Input**: influences (e.g. machining tolerances) from machine model.
6 → **Input**: environmental conditions from building model.
4 → **Input**: influences (e.g. performance level) from human worker model.

Since various processes are required for battery production and different machines can be used, it is not possible to define generic influences which are valid for all processes.

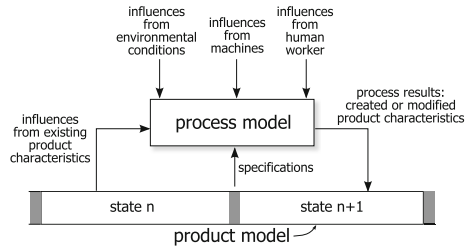
The variations of process results are considered within the multiscale simulation to analyze the impacts of variations in characteristics along a process chain. This consideration allows to evaluate the effects of individual processes on the overall performance of final products. For example, electrodes with different variations in characteristics are assembled into one cell. This effects the performance of each cell. Cells with different performance are combined within one module. Thus, it is important to consider existing characteristics within following processes.

3 → **Input**: existing product characteristics from product model.

Figure 4.20 summarizes the inputs and outputs of a process model. A product model provides information about product specifications and existing product characteristics as inputs to the process model. A process model determines the resulting product characteristics considering process variations based on different process specific

²²The influence of humans in production is relevant if manual activity is required for processing or setup. Since cell production is mostly automated, influences from workers can usually be neglected. In module or system assembly, however, manual assembly tasks may be more relevant.

Fig. 4.20 Process model inputs and outputs



influences (from machines, environmental conditions, and human workers). Furthermore, a process model determines the required machine operation based on product specifications and forwards this information to the machine model. For example, in the mixing process the required time and intensity (in terms of circumferential velocity) determine the operational times and in consequence the production rate as well as the power demand of the mixer.

Output → ②: required machine parameters to related machine model.

Different forms of variation can be observed in battery production (Kenney et al. 2012). First, realized product characteristics can vary between different processing units (e.g. one batch has different characteristics compared to another batch). For example, a created slurry has a viscosity and a solid content which are slightly different to other produced slurries of the same product type. Each batch has only one value for viscosity and solid content. The viscosity of a slurry is – among other factors – influenced by the mixing time, the amount of solvent, and the CB agglomerates. Also there may be interdependencies between those factors. An example is that the viscosity is not much effected by the mixing time if CB agglomerates are already small after dry mixing (Bockholt et al. 2013). Second, variations of a product characteristic can occur within one processing unit. For example, the coating thickness of a coated electrode varies within one batch due to processing tolerances or characteristics of the slurry. Moreover, the mass load in coating is not always constant but can be expressed by a probability distribution (Schmitt et al. 2014). This variation can be assumed to be the same for all batches produced with the same machine setup. Another example is the pore diameter distribution, which indicates variation within a slurry. Third, the variation of product characteristics can occur within and between processing units. An example could again be the coating thickness, which can be different if the machine parameters are slightly changes during setup or due to wear over time. Another example is the assembly of different electrodes with variations in coating thickness into cells. Hence, the capacity of cells depend on the characteristics of installed electrodes. Figure 4.21 illustrates these three forms of variation.²³ The sketched plots show the values for a created characteristic of subsequent processed

²³Figure inspired by a discussion with Fridolin Röder.

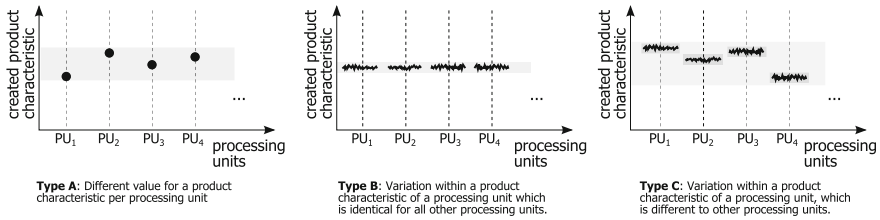


Fig. 4.21 Types of product characteristic variations resulting from one process

processing units for the same process. The grey background shadow indicate the upper and lower limits.

These types of variations determine how product characteristics have to be modeled within a product models. If a process model determines a single value for characteristics (deterministic case or variation of type A in Fig. 4.21), variables can be used within a processing unit to store values. If variation of characteristics occurs within one processing unit (types B and C in Fig. 4.21), arrays have to be used to store multiple values for a characteristic according to a defined resolution (number of values per processing unit). As an example, a processing unit for an electrode batch may contain an array to store values for the coating thickness of defined fractions of the coated foil.

The variation of product characteristics can be determined according to probability distributions (or probability density functions). Examples of distributions are uniform or normal distributions. Distributions can be characterized by its location (e.g. mean or median), spread (e.g. standard deviation or variance), and shape (e.g. skewness). The probability distributions for each resulting characteristic within a process can be determined based on empirical samples or theoretical models.²⁴ So far, process variations from industrial applications have not been published.

Probability distributions or density functions have to be implemented within process models to determine resulting product characteristics. The location, spread, and shape of probability distributions of resulting characteristics may be influenced by previously created characteristics. For example, a higher solid content in the slurry leads to a larger variation in coating thickness. As another example, the viscosity of a slurry is – among other factors – influenced by the mixing time, the amount of solvent, and the size of CB agglomerates. Figure 4.22 exemplary shows possible forms of influences of existing product characteristics on resulting characteristics. In addition, tolerance limits can be defined for each characteristic and if a resulting value lies outside the accepted interval, the processing unit may be classified as waste.

In product and process development, product and process parameters as well as machine configurations are varied and adjusted specifically to achieve a desired result within defined tolerances. Excessively high requirements regarding product characteristics and associated product quality result in very small acceptable tolerances.

²⁴Further information about determining probability distributions and descriptive statistics in the context of product quality can be found for example in Brüggemann and Bremer (2015).

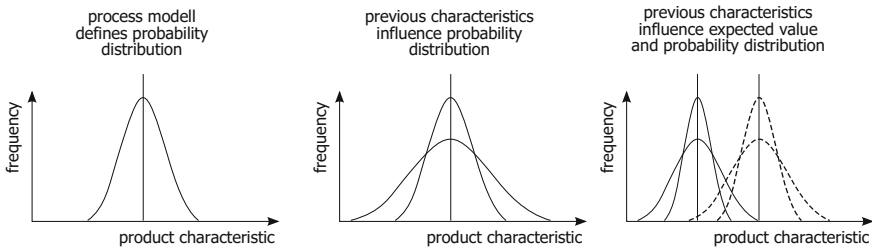


Fig. 4.22 Influences of previous characteristics on probability density functions of created/transformed characteristics

Since the reduction of process variation is associated with increasing complexity and higher costs, unnecessarily small tolerances cause the design and configuration of processes and machines to be more complicated and expensive. Due to the necessary cost reductions in cell production, coordination of process tolerances with required product characteristics as well as detailed understanding and optimization of processes is of great importance. Hence, process models have to be developed considering the type of variation and influences on variations.

Different types of process models can be used within the multiscale simulation. Process models can determine resulting product characteristics and related machine operations in a predictive and deterministic manner. In this case, models hold knowledge about the exact desired value of a product characteristic and the required machine operation (e.g. processing time and intensity). Alternatively, model can use knowledge about process variations to determine the relations between product specifications, existing product characteristics, and external factors on product characteristics. As an example, the relative humidity within the indoor air affects the product quality in the cell assembly. This effect could be described by a parameter model based on empirical experiments or by a physical model if the exact relations between humidity and affected product characteristics are known. However, it is not always possible to find a valid function for each product characteristic. Moreover, often the desired value of a characteristic is known (e.g. from experiments) along with the required process parameter for achieving this value. In this case it is only of interest how the tolerances and variations in the process affect the resulting characteristic. Modeling of the actual physical effects is not necessary. Finally, combinations of different modeling types are possible (e.g. as used by Winter 2016, who developed extensive physical and empirical models to describe the grinding process).

In summary, there are different options for integrating process models for each process into a multiscale simulation:

1. no process model, if no relations are known or relevant.
2. deterministic parameter model, if resulting product characteristics are known (based on specifications) and not subject to disturbances/variation.
3. stochastic empirical parameter model, if variation in process results is known.
4. physical model of theoretical effects on product characteristics.

5. combination of empirical and physical models.

4.4.3 Human Workers (4)

The operation of process chains requires workers for material handling, machine operation and maintenance, as well as for manual assembly tasks. Simulation of humans in production systems enables considering the behavior and characteristics of workers while being active in a production environment. Simulation can be used for different purposes. First, human resources contribute to the production costs (Nelson et al. 2015). Thus, simulation can determine how the number of available workers effects the performance of a process chain. As an example, Halubek and Herrmann (2011) used agent-based modeling of worker behavior and characteristics (e.g. speed, skill level) to examine the worker drift and the resulting performance of mixed-model assembly lines. Second, simulation can be used to determine the effects of humans on the building ambient conditions. Workers move within a factory and emit heat and moisture (ISPE 2009; VDI 2015). These emissions depend on the level of activity of workers which can be represented by different states such as seated, standing, walking, working (Harriman 2002). Heat emissions are relevant since they may influence the air temperature within a building zone which could effect the HVAC operation and the related energy demands. Moisture emissions are relevant if worker operate inside a dry room. In this latter case, emissions of workers increase the humidity of the inside air which may lead to undesired environmental conditions and to higher energy demands for dehumidification. Third, as stated in various studies, worker performance is not deterministic and constant over time but it depends on age, biorhythm, and fatigue of a worker (Siebers 2007; Baines et al. 2004). Simulation could enable to determine the resulting product quality depending on the available workers over time.

Within the multiscale simulation, a worker model represents a worker WO_{wn} as an agent who can move inside and between building zones. Worker activities are coordinated by the process chain model. Workers are required to operate and maintain machines. That means that the process chain model sends requests to worker models about a desired activity. Worker availability and movement times can be integrated into the control strategies of process chains. As an example, a machine can begin to ramp-up only if a worker has arrived.

- ① → **Input:** target position for worker from process chain model.
- ① → **Input:** required activity level from process chain model.

The level of activity of each worker can be represented by a state chart as shown in Fig. 4.23. The chart differentiates the states seated at rest, walking slowly, light work, medium work, and heavy work. If a worker is inactive, the agent is in the state seated at rest. If a worker is called to operate a machine, the worker moves

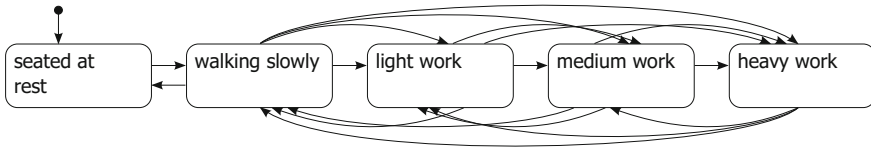


Fig. 4.23 State chart of worker activity

with a defined velocity towards the machine. At a machine, the intensity of work depends on the machine type and machine state (e.g. required is medium work during machine setup and light work during processing for machine supervision). Each state is associated with values for heat and moisture emissions. Detailed information about heat and moisture emissions of humans can be found for example in Bohne (2014) and Harriman (2002).²⁵ The heat and moisture emissions are provided to the process chain model since it aggregates all emissions for each building zone.

- Output** → ①: heat emissions $\dot{Q}_{WO_{wn}}$ to process chain model.
- Output** → ①: moisture emissions $\dot{M}E_{WO_{wn}}$ to process chain model.

In order to allocate the emissions to a building zone, the process chain model has to know the position of each worker within the shop floor coordinate system.

- Output** → ①: current position of worker WO_{wn} to process chain model.

Overall, simulation of human worker activities can enable the analysis of the impacts on process chain operation, product quality, heat and moisture emissions as well as on labor costs. However, the impacts of workers on total energy demands for cooling and dehumidification as well as on total production costs is relatively small.

4.4.4 TBS Models (5)

Relevant TBS systems for battery production are lighting, compressed air generation, and systems for ventilation, heating, and air conditioning. These systems have to be modeled and integrated in the multiscale simulation. The purpose of these models is to

- describe the operation of TBS systems depending on the process chain operation,
- determine the energy demands of systems and their share of the total energy demand of the production system,
- identify energetic hot-spots for the derivation of improvement measures regarding dimensioning or control of TBS, and to

²⁵For example, heat emissions range from 95 W (seated at rest) to 270 W (hard work).

- understand and describe interdependencies between production system elements and TBS systems (e.g. correlations between dry room conditions and product characteristics).

4.4.4.1 Lighting

Lighting requires electrical energy and emits heat to the building which may cause additional cooling loads for the air conditioning. Both the energy demand and heat emissions (both in W/m^2) depend on the light intensity LI_z of a building zone (in lm/m^2), the efficiency of lamps LE_z (in lm/W), and the duration.

It is assumed that lights in a zone are on if workers are inside the zone, if machines are operating, and if available daylight is not providing sufficient illumination. The schedules for lighting depend on the process chain operation. For example, the lights in a zone are turned on when the first worker enters the zone and turned off if the last worker leaves and no machine is operating. The lighting model uses the two states on and off for lighting control and determines a constant power demand based on LI_z , LE_z , and the zone area A_z . The model generates the power demand profile of lights based on the schedule provided by the process chain model.

1 → **Input:** signals for turning lights on and off from process chain model.

The total power demand of lighting is calculated by summing up the power demands of all light sources in all building zones. The total power demand is provided to the process chain model.

Output → **1**: power demand PD_{LIGHTS} to process chain model.

The required power is emitted as heat to the related building zone (Hesselbach 2012). The resulting heat emissions are provided to the process chain model.

Output → **1**: heat emissions \dot{Q}_{LIGHTS} to process chain model.

The proposed lighting model is kept rather simple. More detailed models are possible if lighting has strong influence on the production processes or if the energy demand contributes to a high share of the total energy demand. Ryckaert et al. (2010) provide a detailed discussion of energy efficiency measures for lighting. They proposed a model to determine the required power considering LE of a zone and different task areas with specific requirements.

4.4.4.2 Compressed Air Generation

Compressed air is used to transform electric energy into mechanical energy. It is among the most expensive and least efficient forms of energy²⁶ (Mousavi et al. 2014) and a high share of industrial energy demands is caused by compressed air generation (Ruppelt 2003). For this reason, a model of a compressed air generation system is proposed for the multiscale simulation. The purpose of this model is to examine the impacts of system configurations and control strategies on the power demand PD_{CAS} and pressure cap – similar to Mousavi et al. (2014) and Thiede (2012).

A compressed air generation system usually consists of components for generation (one or several compressors), preparation and treatment (e.g. filters), and distribution (e.g. tank, pipes) of compressed air. Such system can supply multiple consumers (e.g. machines) within a process chain. The proposed modeling concept focuses on the power demand of compressors since compressors are the main component of a system supplying air to generate the desired pressure. The model must enable to simulate the system pressure and the related operation of compressors.

The condition of compressed air is defined by pressure (p), volume (V) and temperature (T) according to the following relation (Bierbaum and Hütter 2004).

$$\frac{p \cdot V}{T} = constant \quad (4.16)$$

A common simplification for the determination of the system behavior is the assumption of an isotherm process.

$$p_0 \cdot V_0 = p_1 \cdot V_1 = constant \quad (4.17)$$

The flow of air can be described by the amount of air flowing through a cross section during a specific period of time which can be specified as volume flow (\dot{V}). The pressure cap within the compressed air system with volume V_{CAS} depends on the inside volume change caused by air supply from the compressor(s) (V_{in}) as well as demand from machines and pressure losses (V_{out}).

$$cap = \frac{V_{CAS} + V_{in} - V_{out}}{V_{CAS}} \quad (4.18)$$

The demand from machines is determined within the process chain model by summing up the compressed air demands of all machines.

1 → **Input:** compressed air demand CAD_{MACH} from process chain model.

²⁶The efficiency of compressed air generation can be increased by measures such as heat recovery and adjusted compressor control (Saidur et al. 2010).

The system pressure has to be kept within a defined interval. If the pressure decreases below pressure cap_{min} , air is supplied to the system until the maximal pressure cap_{max} is reached. Different control strategies exist for compressors (Bierbaum and Hütter 2004). The objective of the controller is to maintain the desired system pressure while minimizing energy demand and component wear. The controller directly affects the air supply and the power demand of compressors. For simplification of the model, it is assumed to use only one compressors which is able to supply the desired supply rate.²⁷ The controller determines if the compressor is in off, on, or idle state. Within each state, the compressor has a specific power demand. An example of a control strategy is the intermittent control using a two-point controller. The compressor is switched on if $cap = cap_{min}$ and turned off if $cap = cap_{max}$. Other control strategies – for example keeping the compressor in idle state until shutdown – are explained for example in Bierbaum and Hütter (2004) and Ruppelt (2003). The resulting power demand of the compressor is assumed to equal the power demand PD_{CAG} of the compressed air system ($PD_{CAG} = PD_{comp}$).²⁸ The power demand as well as the system pressure are provided to the process chain model. The latter allows machine models to check if the available system pressure is sufficient for machine operation.

Output → ①: power demand PD_{CAG} to process chain model.

Output → ①: system pressure cap to process chain model.

This model of a compressed air system allows determining the power demand of compressors and the pressure based on the compressed air demands of machines from a process chain. If required, the model can be extended towards considering multiple compressors with individual characteristics and other system components.

4.4.4.3 HVAC

The indoor climate of a production facility has to be controlled according to process requirements and comfort of workers. Furthermore, the exhaust air of a facility has to be cleaned from substances which are harmful to the environment. For this purposes, HVAC systems are installed for ventilation, heating, and air conditioning (cooling, humidification, dehumidification) of buildings. Usually, an air handling unit (AHU) is installed for each building zone which is equipped to fulfill the required treatment functions (Bohne 2014). The required environmental ambient conditions within a facility for battery production are described by Simon (2013). Since HVAC systems may account for up to half of the energy demand in a facility (Pérez-Lombard et al.

²⁷Often also several compressors (of the same or different types) or multi-staged compressor systems are used to meet the maximum switching operations for each compressor, to supply air with different rates, or to achieve higher system pressures. The model can be adjusted accordingly.

²⁸More detailed models may also include the power demands of filter, dryers or other equipment.

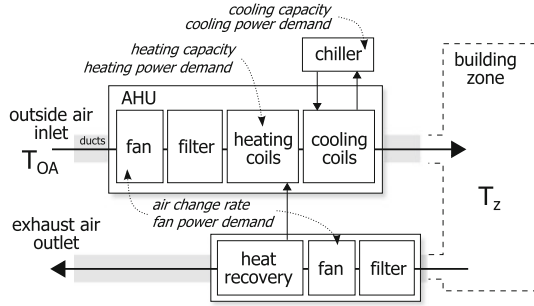


Fig. 4.24 Schematic of an exemplary HVAC system for a building zone equipment for ventilation, cooling and heating with heat recovery

2008), it is relevant to model the operation of these systems and to consider the energy demands in the evaluation of battery production.

Ventilation, Heating, and Cooling

The inside air within a building zone is exposed to various emissions from processes, humans, materials, etc. These emissions reduce the air quality and require ventilation with outside air according to an air change rate acr^{29} (Fitzner 2013). In order to maintain the desired air quality in production facilities, AHU for ventilation usually consist of an outside air inlet, a central processing unit with fans and filters, and ducts for air distribution to the air outlets into the building zone. Detailed descriptions of various types of AHU are given in Bohne (2014) and Fitzner (2013).

Furthermore, a building is subject to internal and external heat sources and sinks. Depending on specific heat flows and dampening effect of thermal masses inside a building zone, heating or cooling equipment may have to be used in addition to ventilation in order to establish the desired indoor temperature. In this case, AHU have to be equipped with heating and cooling coils as well as external chillers supplying the cooling coils (Bohne 2014). The controller of an AHU for heating controls the operation of these different components according to setpoint temperature values and sensor signals of current indoor (T_z) and outside (T_{OA}) air temperatures. Figure 4.24 shows a simplified and abstract schematic of an exemplary HVAC system for ventilation, heating, and cooling with heat recovery.

If the inside air temperature in a zone is too high or too low, the supplied air has to be heated or cooled in order to adjust the inside air temperature to the desired value. The heating and cooling demands depend on the outside air temperature which depends on the season and location of a facility. To give some examples, Fig. 4.25 shows the daily mean temperatures for three locations.³⁰ The figure allows to con-

²⁹The air change rate defines how often the air within a zone has to be changed during one hour.

³⁰Reno is the location of the Tesla giga factory for battery cells, Braunschweig is the location of the Battery LabFactory Braunschweig, and Iceland is basically a rather cold country.

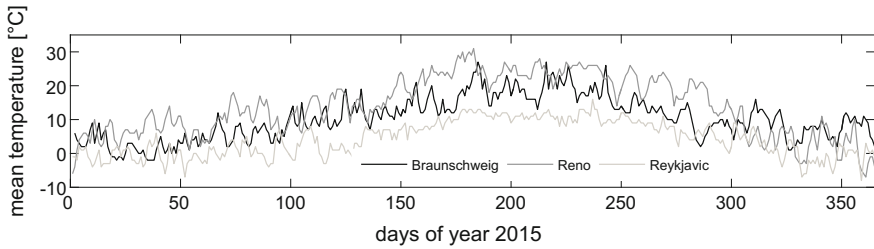


Fig. 4.25 Daily mean temperature [°C] in Reno (Nevada, USA), Braunschweig (Germany) and Reykjavik (Iceland) in 2014 (based on data from Weather Underground 2015)

clude that the heating and cooling demands for buildings at these locations differ according to the outside temperatures.

Simulation models of HVAC systems for ventilation, heating, and cooling should enable to determine the operation and energy demands of AHU equipment considering internal (e.g. heat emissions of machines or humans) and external (e.g. outside temperature) influencing factors. In contrast to static calculations of maximum heating and cooling loads (required for system design), simulation allows analyzing the dynamic behavior of AHU in different situations and a more precise determination of energy demands. For this purpose, the inside and outside temperatures have to be considered in the simulation. Furthermore, the simulation has to imitate different time periods in order to account for seasonal conditions.

⑥ → **Input:** indoor temperature of building zone from building model.

⑥ → **Input:** outside weather conditions from weather file.

Based on this information, models of HVAC components determine the required heat flows for heating or cooling for each zone and the resulting power demand.

Output → ⑥: heating or cooling loads \dot{Q}_{HVAC_z} to building model.

Output → ①: power demand PD_{HVAC} to process chain model.

These values depend on the implemented control strategy of the AHU components (e.g. two-point or variable heat flow control) and the setpoint values (e.g. accepted temperature interval).

Dehumidification

In addition to defined indoor temperatures, some processes of battery cell assembly have to take place in dry room conditions with very low humidity. The humidity of the inside air is influenced by the humidity of the supplied air, leaks in the dry room

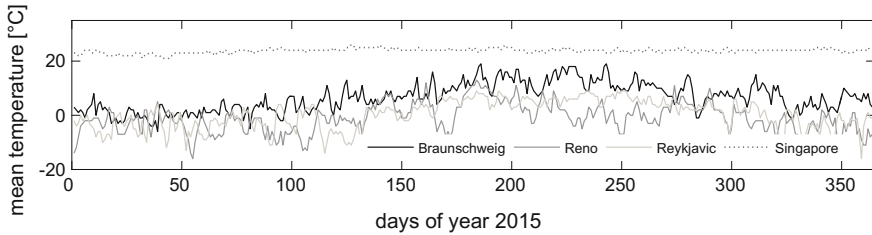


Fig. 4.26 Daily mean dew point temperature [°C] in Singapore, Reno (Nevada, USA), Braunschweig (Germany) and Reykjavik (Iceland) in 2014 (based on data from Weather Underground 2015)

constructions, and internal moisture gains from humans³¹ or products (Harriman 2002). In order to achieve very dry conditions, an AHU of a dry room has to be equipped with a dehumidification system – in addition to the HVAC components for ventilation, heating and cooling – which removes humidity from the supply air.

In production facilities of battery cells, commonly used are desiccant dehumidification units (Harriman 2002). Within AHU with such units, the inlet air stream is mixed with a circulating air stream from the dry room and cooled down before dehumidification. Within the desiccant dehumidification unit, the moisture of the inlet air stream is transferred to a regeneration air stream, which is heated before entering the dehumidifier to enable a high intake of moisture. This regeneration air stream is transported to the outside of the building (Harriman 2002). After dehumidifying, the inlet air stream is heated before entering the dry room. The energy demands of an AHU for dehumidification depend on internal heat and moisture emissions as well as on outside air conditions such as temperature and humidity. The humidity of the outside air can be characterized by the dew point temperature³² which also depends on the location of the facility. To give some example, Fig. 4.26 shows the daily mean dew point temperature for four different locations for 2014. In addition to the locations selected for Fig. 4.25, Singapore was added due to its high dew point temperature. The figure allows to conclude that the location influences the energy demand of dehumidification systems.

Consequently, models of HVAC systems for dehumidification must – in addition to the described influences on ventilation, heating, and cooling – consider the humidity of the outside air as well as the moisture emissions within a dryroom building zone which increase the humidity of the inside air.

6 → **Input:** outside weather conditions from weather file.

³¹Harriman states that humans adapt to very low humidity levels and cause lower moisture loads in super-dry conditions such as found for example in battery production.

³²The dew point temperature is the temperature at which the contained water is condensed into water. It also defines how much vapor is contained in the air.

Since HVAC systems can be of various types (e.g. with or without circulating air flow, heat exchange, or dehumidification), it is not possible to derive a generic HVAC system model. Models have to be created specifically for a HVAC system under examination. For this purpose, different generic models and tools for HVAC simulation have been developed. For example, Chen and Treado presented a library for physical modeling of different HVAC components (Chen and Treado 2014). De Antonellis et al. developed a detailed model for the simulation and optimization of a desiccant wheel (De Antonellis et al. 2010). Furthermore, different libraries are available which allow to use predefined components to design simulation models of HVAC systems with the software environments Modelica (e.g. Wetter et al. 2014) or Simulink (e.g. Kalagasidis et al. 2007). However, despite this preliminary works, physical modeling of HVAC systems is still no easy task. As an alternative to physical modeling, models for HVAC systems can also be derived from empirical data as shown by Cherem-Pereira and Mendes (2012) for the example of room air conditioners. If measurements about the power demand of different components as well as the related environmental conditions are known, such approach may be of sufficient accuracy for the modeling of the HVAC system operation.

Overall, the simulation of HVAC systems is closely connected to the simulation of the thermal response of buildings since inside ambient conditions are the controlled variables in HVAC system controllers. Various research approaches were already developed for the integrated or coupled simulation of HVAC systems and buildings, for example Noudui and Wetter (2014), Zuo et al. (2014), Gorecki et al. (2015), Feng et al. (2012), Wetter (2010), or Trčka and Hensen (2010). Consequently, a building model is also needed for the proposed multiscale simulation to determine the inside ambient conditions of a battery production facility and the impacts on HVAC systems.

4.4.5 Building Model (6)

The building shields the production system from the outside environment. A building can usually be divided in one or multiple thermal zones which can have different properties, thermal behavior (e.g. losses or heat capacities) and desired inside ambient conditions. These inside conditions depend on the building properties (e.g. structure, shape, number of floors, windows, orientation, location, and materials) and various external and internal influences. The purpose of building simulation models is to determine the inside conditions of specific building zones based on these external and internal influences (VDI 2001). Thermal simulation enables analyzing the relevant influences and if passive improvement measures (e.g. sunscreens) allow to reduce the HVAC system operation while maintaining the desired conditions (Bohne 2014; Hesselbach 2012). In the multiscale simulation, the results of the building simulation are inputs to HVAC models as well as to process models in case the environmental conditions have influence on the processing results.

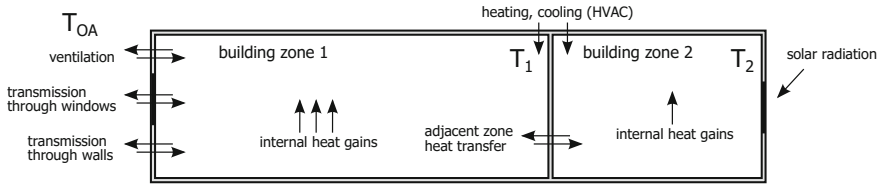


Fig. 4.27 Simplified heat flows of an exemplary two-zone building

Output → 5: inside conditions of building zones to HVAC models.

Output → 3: inside conditions of building zones to process models.

The determination of inside conditions is based on the analysis of heat losses and heat gains (energy flows) through the building shell and between building zones. Heat losses can be divided into transmission losses and ventilation losses. Heat losses due to transmission \dot{Q}_{tr} are influenced by the wall surface area A_w of a zone. Furthermore, they are influenced by heat transfer coefficients U_w of the materials of the surrounding walls and by the difference between the inside and outside air temperatures.³³ Heat losses due to ventilation \dot{Q}_v are mainly influenced by the air change rate acr .³⁴ External heat gains can also be caused due to transmission and infiltration through the ventilation system. Furthermore, heat gains are caused by solar radiation \dot{Q}_s through windows.³⁵ Internal heat gains are caused by the HVAC air supply (heating or cooling) \dot{Q}_{HVAC} , as well as by heat emissions from machines \dot{Q}_{MACH} , lights \dot{Q}_{LIGHT} , and workers \dot{Q}_{WO} . Figure 4.27 illustrates exemplary heat flows related to a building with two zones.

The inside temperature T_z of a building zone can be calculated based on the energy balance.

$$\dot{T}_z = \frac{\dot{Q}_s - \dot{Q}_{tr} - \dot{Q}_v + \dot{Q}_{HVAC} + \dot{Q}_{MACH} + \dot{Q}_{LIGHTS} + \dot{Q}_{WO}}{m_{air} \cdot c_{air}} \quad (4.19)$$

The calculation of heat flows due to transmission, ventilation and radiation requires information about the outside temperature which can be taken from radiation models and weather data. Established weather data sources are files created based on the test reference year (TRY) method in which meteorologists define an average year for different locations (Fitzner 2013).

The values for internal gains are determined by HVAC models, machine models, worker models and by the lighting model. They are aggregated within the process chain model.

³³ $\dot{Q}_{tr} = \sum_w U_w \cdot A_w \cdot (T_z - T_{OA})$, (Hesselbach 2012).

³⁴ $\dot{Q}_v = acr \cdot m_{air} \cdot (T_z - T_{OA})$, (Hesselbach 2012).

³⁵ $\dot{Q}_s = A_d \cdot I_{max} \cdot g$; with window area A_d , maximum radiation I_{max} , and energy transmittance g , (Bohne 2014).

- 5 → **Input:** heating or cooling loads \dot{Q}_{HVAC_z} from HVAC model.
- 1 → **Input:** aggregated heat emissions \dot{Q}_{TOTAL_z} from process chain model.
- 1 → **Input:** aggregated moisture emissions \dot{ME}_z from process chain model.

The process chain model has to contain information about the zones of a building to allocate the heat emissions. That includes also heat emissions from moving objects such as processing units (not relevant in battery production) and workers (Wright et al. 2013).

Assessing the detailed thermal response of a complete building requires simulation³⁶ (Bohne 2014) with physical models to analyze the effects of different weather conditions and scenarios (e.g. shifts). Crawley et al. presented an overview of the capabilities of existing building simulation tools (Crawley et al. 2008).

4.5 Model Connection (7)

The derived models have to be connected in order to realize a multiscale simulation imitating the dynamic behavior of an entire production facility. In this context, there are two main tasks: The clear definition of interactions and information exchange between models as well as the selection of suitable strategies for coupling and synchronization of the involved models (which have been implemented in a software).

Interactions and Information Exchange

Interactions and information exchange depend on the desired input and output variables of models. Models providing specific variables have to be connected with models in need of these variables. The relevant inputs and outputs of different model types have already been indicated during the derivation of models. Figure 4.28 illustrates the resulting proposed multiscale model structure and the interactions between models (output ■ → □ input). This illustration refers to a generic case but can be adapted to any type of production system (according to the defined system boundaries) by adding of models for specific machines, processes, and products. For a specific multiscale application, it is necessary to identify all required variables of all involved models. This includes units and resolutions of each variable along with the required frequency of updated values. Furthermore, it is important to optimize the routing of information flows since every interface between two models causes efforts for implementation and the risk of errors or information loss (e.g. due to rounding or different model resolutions). For this reason, the process chain model is suggested to

³⁶Alternatively, static calculations can be applied (Hesselbach 2012). Static approaches utilize performance indicators, standardized factors or metrics to determine stationary energy balances of buildings. Static calculations can determine the expected heating or cooling demands for extreme weather conditions at a given location. The results can be used for the design and dimensioning of HVAC systems.

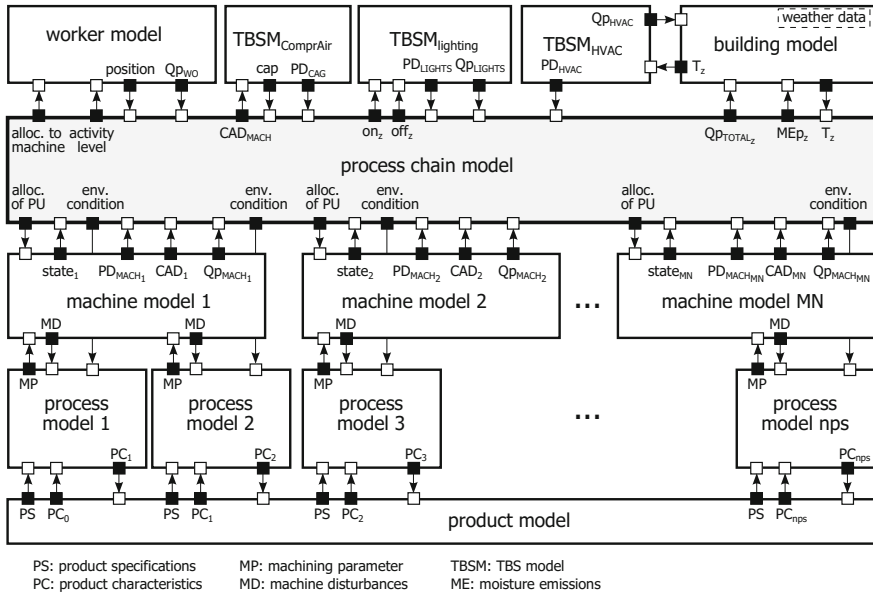


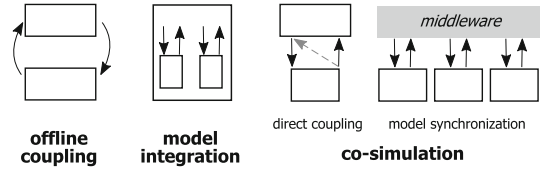
Fig. 4.28 Structure and exchanged variables of total multiscale model

act as a coordinator which collects, aggregates, and distributes information to other models. As an example, the process chain model collects heat emissions of machines, lights, and workers, aggregates these to total heat emissions per building zone, and delivers this information to the building model. The building model in return provides the inside temperature for each building zone to the process chain model which distributes this information to machine and process models. This structure simplifies the information flow, reduces the number of interfaces between models and creates flexibility towards the addition of new models.

Coupling and Synchronization

The actual coupling of models can be realized according to different concepts of which the most relevant for production simulation are offline coupling, model integration and co-simulation (Ören 2014; Brecher et al. 2009). Figure 4.29 illustrates the different coupling concepts. Offline coupling means that coupled models are executed sequentially and that results are exchanged after each simulation run of one model. Although this type of coupling is relatively easy to implement, it is not suitable for the proposed multiscale simulation approach since it is not possible to consider dynamic interactions between models during simulation runs. Integration of models means that different models are implemented within one integrated model in the same software tool to avoid data exchange and synchronization between different tools. Models exchange data at each simulation time step or at certain events. In co-simulation, models are implemented in specialized simulation environments which are connected to each other. The data exchange has to be synchronized since

Fig. 4.29 Concepts for coupling of models (from left to right): offline coupling, model integration, and co-simulation (direct coupling and model synchronization)



simulation times of individual models may differ. The time between two synchronization steps must be adjusted according to the modeled system behavior. A short synchronization time may reduce the simulation execution performance while a long synchronization time could effect the simulation results because updated variables may be synchronized too late. If interactions between only two models have to be considered in co-simulation, these models could be directly coupled via a specific interface. In this case, one of the models is responsible for the synchronization. If data exchange has to be synchronized between several models and software environments, this can be realized by using coordinating middleware software based on principles of HLA or other middleware solutions (e.g. TISC (Kossel et al. 2006)).

These coupling concepts can also be combined. For example, generic machine models and product models can be integrated into a process chain model and process models can be directly coupled to machine models. The process chain model can be synchronized with detailed machine models and models for HVAC systems, compressed air generation, and a building.

In summary, the connection of models allows to execute and coordinate all models of a multiscale simulation and to simulate the dynamic interactions between the modeled production system elements. The simulation results of each model have to be combined in order to support the desired planning tasks and decisions. For this purpose, it is suggested to determine and prepare the desired results within the process chain model since it has access to data from all other models.

4.6 Result Evaluation and Visualization (8)

The resulting large amount of generated data during simulation has to be examined with respect to the overall performance of the production system. The results allow deriving detailed insight into the cause-effect relations between machines, TBS systems, processes and product characteristics, as well as the material flow. Such detailed analysis is needed to avoid problem shifting which may occur by only considering isolated system elements of a production facility or planning perspectives. Consequently, the simulation results of different models can be combined and aggregated to performance indicators for a consistent evaluation of improvement measures and the enhancement of the production system understanding.

Variables and Indicators

Simulation results can be related to the overall performance of a production system, process chains, single machines, jobs, or processing units. For an entire production system, relevant indicators are the total energy demand and the energy demands of different systems such as machines, HVAC systems, compressed air generation, lighting, etc. This allows the identification of the most relevant systems with high energy demand. In addition, the overall material consumption is of interest, divided in raw materials for products and auxiliary materials required for production. The energy and material demands can also be related to the output of final products (e.g. in GWh of battery cells) during a period of time. These indicators on system level enable deriving total costs and environmental impacts of the production activity and comparing of different simulation runs. For example, the production costs C_{total} can be determined by considering the total energy demand per energy carrier along with energy prices based on the supply contract (C_{energy}), the consumed amount of materials along with the unit prices for each material type ($C_{materials}$), and the total costs of machine operation based on the operational time of each machine and the related machine-hour rates ($C_{machining}$).

The total environmental impacts of production EI_{total} can be determined based on the total energy demand per energy carrier along with the related environmental impacts per energy carrier (EI_{energy}) as well as the used amount of materials together with the related environmental impacts of each material type per kg ($EI_{materials}$). In general, the environmental impacts can be expressed regarding different impact categories. A commonly used indicator is the GWP which describes the induced contribution to climate change (Thiede 2012). In this regard, equivalent CO₂ emissions caused by energy and material production can be applied as an indicator for the environmental impacts on system scale. However, in order to gain insight into the dynamic production system behavior and to evaluate specific improvement measures, required is a more detailed evaluation of the performance of production system elements.

The material flow characteristics of process chains determine the output of semi-finished and finished products as well as the operation of machines and related systems. More specifically, a process chain can be characterized by its yield of product units per product type, its utilization, as well as by the average production lead time of all jobs per product type. Furthermore, the energy and compressed air demands, non-productive time and energy demand shares, and heat emissions of all machines can be aggregated to identify critical machines or associate processes.

The operation of individual machines is influenced by the material flow within a process chain and it can be evaluated based on indicators for energy demands and utilization. Energy demands can be derived by values of the state depended electrical power demand and the compressed air demand. The utilization is determined by the ratio of productive and non-productive time shares. A machine is only considered productive within the processing state. If a machine is in setup, blocked or failure state, it is considered non-productive. In addition, the overall heat emissions of a

machine can be calculated for a given period of time to study the effects on HVAC systems operation.

While the process chain model generates performance indicators about the material flow of all jobs which are completed during a time period, single jobs and processing units collect data about their specific material flow as well as specific energy and material demands. Indicators of a job depend on the indicators of the associated processing unit(s). Relevant indicators describe the start and finish time, lead time, non-productive time share, and times per machine. Furthermore, relevant results are the specific energy demand and material input per material type per processing unit. They allow deriving the direct material costs and costs of machine operation based on machine-hour rates. Material costs can be represented by a cumulative plot in order to indicate the value of a semi-finished processing unit during production. Finally, processing units store information about created or modified product characteristics. Jobs can aggregate the product characteristics of all associated processing units as average values or represented by a histogram. Also, on process chain level, the product characteristics of processing units of all jobs (of one product type) can be characterized by their distributions. This enables identifying the spread of individual product characteristics and the origins of variations.

Table 4.3 lists all suggested performance indicators with units and suitable forms of representation. These indicators have to be made accessible by a simulation tool or available within generated reports.

Value Stream Representation

In addition to single performance indicators, each job and processing unit can be described by a value stream map. Value stream mapping (VSM) is an established method aiming at the identification of inefficiencies and waste within a production line (Erlach 2007). Value stream maps illustrate the processes required for production along with buffers and specific process data. Traditional VSM focus on the identification of lead times and non-value adding time shares but it was already extended toward the consideration of specific energy demands (EVSM) for a job or per product unit (Erlach and Westkämper 2009; Bogdanski et al. 2013). Figure 4.30 illustrates the structure for an extended EVSM representation of the simulated flow and processing of a processing unit for a battery cell. In general, the application of VSM requires relatively low effort and the visualization of results is easy to understand even without having expert knowledge. However, shortcomings of the traditional static VSM method are that a value stream map refers to one product type or family and that it is based on one time measurements or average values. Thus, a value stream map has a snapshot character and it is not possible to consider dynamic interactions between different jobs such as blocking of machines which may cause waiting times. This shortcoming is abolished in the multiscale simulation since value stream maps can be dynamically created for each job and processing unit. The model is able to trace the material flow of processing units by creating a data box representation to each processing unit with simulated values for times, direct and indirect energy demands, and material demands for each completed process. This simulation of value stream maps is based on the Multi-product EVSM (MEVSM) approach

Table 4.3 Result indicators for different scales of production systems

Reference	Indicator	Unit	Suggested representation
Production system	Total energy demand ED_{TOTAL}	kWh	Number
	Energy demand per energy carrier	kWh	Number
	Total power demand PD_{TOTAL}	kWh	Plot
	Energy demand of TBS ($ED_{CAG}, ED_{HVAC}, ED_{LIGHTS}$)	kWh	Numbers
	Share of energy demand per machine/system	kWh	Pie chart
	Output of final products		Number
	Total consumption of raw and aux. materials	kg	Numbers
	Energy costs per energy carrier	EUR	Numbers
	Total energy costs C_{energy}	EUR	Numbers
	Material costs (for all material types) $C_{materials}$	EUR	Numbers
	Costs of machine operation $C_{machining}$	EUR	Numbers
	Total production costs C_{total}	EUR	Numbers
	Environmental impact of energy supply EI_{energy}	kg CO_2^{eq}	Numbers
	Environmental impact of material consumption $EI_{materials}$	kg CO_2^{eq}	Numbers
Total environmental impact EI_{total}	kg CO_2^{eq}	Numbers	
Process chain	Utilization uti_{PC}	%	Number
	Output/yield of product types Y_t^{pin}		Numbers
	Energy demands per machine	kWh	bar/pie plot
	Compressed air demands per machine	m ³ /h	bar/pie plot
	Waiting times per machines	s, min	bar/pie plot
	Blockings per machine		bar/pie plot
	Heat emissions per machine per zone	kWh	bar/pie plot
Machine	Utilization uti_{mn}	%	Number
	Energy demand $ED_{MACH_{mn}}$	kWh	Number
	Power demand $PD_{MACH_{mn}}$	kW	Plot
	Compressed air demand $CAD_{MACH_{mn}}$	kW	Plot
	Share of productive and non-productive times	%	Pie chart
	Share of productive and non-productive energy demand	%	Pie chart
	Total heat emissions $\dot{Q}_{MACH_{mn}}$	kWh	Number

(continued)

Table 4.3 (continued)

Reference	Indicator	Unit	Suggested representation
Job and processing unit	Lead time	s, min	Number, VSM
	Start time (overall, per process)	s, min	Number, VSM
	Finish time (overall, per process)	s, min	Number, VSM
	Share of productive and non-productive times	%	Pie chart, VSM
	Material input per material type	kg	Number
	Material cost	EUR	Number, cumulative plot
	Material cost per material type	%	Pie chart
	Material cost per process	EUR	Number, VSM
	Direct and indirect embodied energy (<i>iee, dee</i>)	kWh	Number
	Embodied energy per process	%	Pie chart, VSM
Product characteristics	Various	Numbers, histograms	

(Schönemann et al. 2016). The MEVSM approach combines VSM and simulation by using a generic structure for the definition of product type specific routing, product characteristics³⁷, and process parameters, as well as an AB and DE simulation logic which allows calculating process specific performance indicators and product specific evaluations. Using the MEVSM approach enables generating value stream maps for all processing units which are produced simultaneously within one process chain. A similar approach is the E²VSM approach which also combines DE simulation with VSM to generate economic and environmental evaluations of the production of multiple product types (Alvandi et al. 2016).

Furthermore, for the simulation of battery production, the simulated value stream map representation can be modified to show material inputs with related material costs and costs of machine operation. Additionally to the VSM representation of jobs or processing units, this kind of representation can be used for all jobs of each product type combined. In this case, the values in data sets per process have to be replaced by the average values determined by the values of each job. Moreover, a histogram could be given for each data item, for example showing the direct energy demands of all electrodes for coating and drying. This representation allows identifying the most time or energy intensive production step of each product type.

Evaluation of stochastic effects

³⁷Details about integrating product characteristics into value stream modeling are discussed in Schönemann et al. (2014).

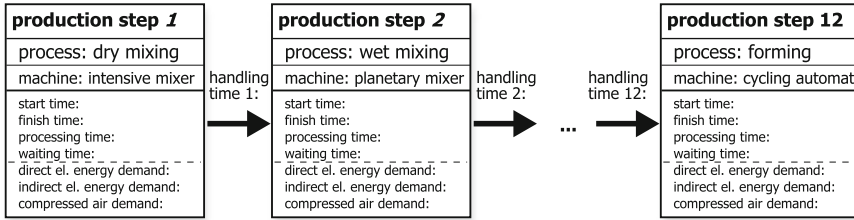


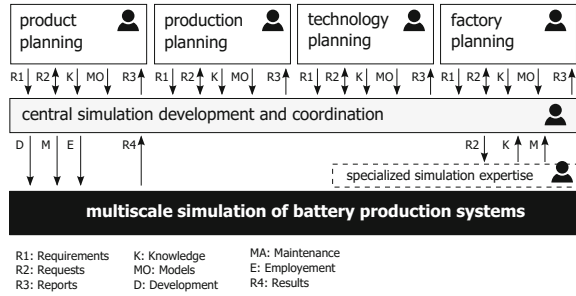
Fig. 4.30 Structure for an extended value stream representation of the production of a processing unit for a battery cell

If variables or inputs of a simulation model are stochastically distributed, the results also have to be considered as random variables. In this case, simulation runs represent sampling experiments with fluctuating outcome. Random variables have to be described using descriptive statistics. That means that they have to be represented by expected values and measures for variation. Within the result presentation, histograms or box plots can be used to show the distribution of resulting values. Furthermore, it is necessary to determine the minimum number of simulation runs required to achieve statistically significant results (e.g. for a Monte Carlo simulation). Detailed information about dealing with uncertainty are given for example in Rabe et al. (2008) and Liebl (1995).

4.7 Application Procedure

The development and employment of a multiscale simulation is different compared to monolithic specialized models. It allows to combine the knowledge and expertise of different engineering disciplines. In particular, the improvement of battery production regarding product quality, costs, and environmental impacts demands the cooperation of the planning of products, processes, production technology, and factories. These disciplines have their own planning tasks and often use isolated tools or models for the evaluation of specific measures. The knowledge from these disciplines and the available models have to be combined for creating the proposed multiscale simulation. However, existing specific models are often not compatible or reusable by other disciplines (Bergmann 2014). For this reasons, a central function for simulation development and coordination is required which collects and adapts existing models and knowledge for the use in a multiscale simulation. Furthermore, this central function is responsible for the employment of the multiscale simulation and for the generation of reports which are tailored to the needs of the involved disciplines. However, the involvement of all stakeholders and disciplines into the modeling process is essential to foster learning effects and an interdisciplinary system understanding. Once a multiscale simulation environment is developed and established, each discipline can file requests for simulation results related to a specific objective. The central function will adapt the simulation accordingly and perform simulation runs to generate reports. If objectives require more detailed simulation models of which

Fig. 4.31 Structure for development and employment of a multiscale simulation with the involved disciplines



no expertise is available within the involved stakeholders (e.g. for detailed building simulation), specific simulation expertise has to be (externally) acquired in order to integrate the desired model functions. Figure 4.31 shows the described structure of cooperation of disciplines for the development and employment of a multiscale simulation.

There are multiple ways to apply the developed simulation concept to a specific simulation environment. Different objectives, the availability of simulation models, the know-how of simulation engineers, as well as other organizational and technological factors (e.g. available personal resources or software) can influence the application to a large extent. However, a generalized application procedure should help simulation engineers to structure the development process for a multiscale simulation. This application procedure is divided into twelve steps which are structured in six phases similar to simulation study procedures proposed by Banks et al. (2010) or Wenzel et al. (2008). Figure 4.32 illustrates these phases and steps and also the areas of involvement of stakeholders from different disciplines. The simulation development and coordination function is responsible for planning, realization, and controlling of the twelve-step procedure. The other disciplines support during problem formulation and provide specific planning objectives which should be supported by the simulation. Also they are involved in the development of specific models and the final evaluation of the simulation results. The specific tasks and methods for the twelve steps of the procedure are described within the next subsections.

4.7.1 Description of Production System and Stakeholders (I)

In the first step, the battery production system under survey has to be described along with the roles of involved stakeholders. This is important for clarification of the context for the simulation and the following definition of objectives. The description has to refer to the production stage (e.g. cell production and/or system assembly), product variety, industrial scale (e.g. production volume per year), and utilized production technology. Moreover, the description has to clarify the responsibilities and organizational structure of different disciplines, departments, and people. A result

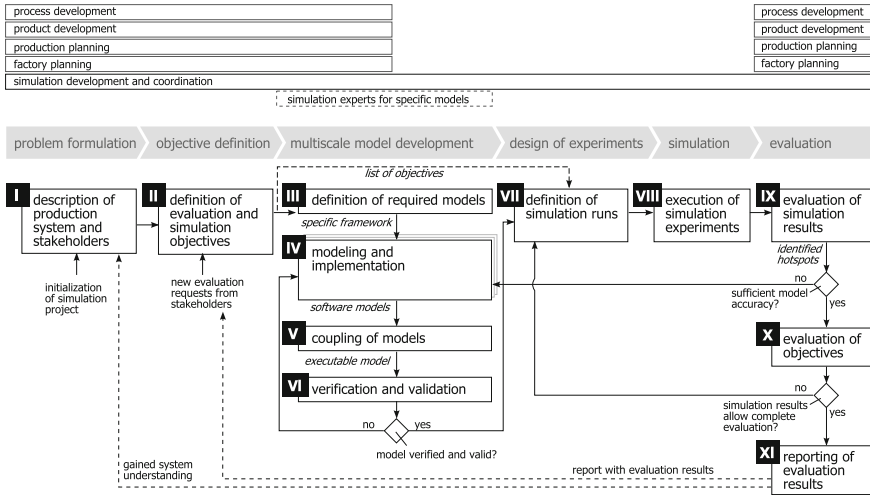


Fig. 4.32 Procedure for application of the multiscale simulation concept

of this first step is a definition of the system boundaries and the responsibilities for model development as well as the specific use cases of the simulation.

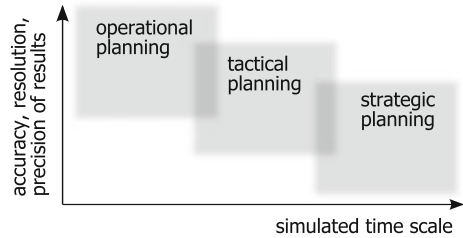
4.7.2 Definition of Evaluation and Simulation Objectives (II)

In addition to this greater objective, it is necessary to specify the strategic, tactical or operational planning perspective in order to derive the required accuracy and scope of the simulation results.

Strategic Strategic decisions – such as investment in a new production facility – face a higher degree of uncertainty and demand the analysis of aggregated effects for a longer time period of the simulated production system operation (e.g. a full year to consider seasonal effects of the local climate). The purpose of a simulation study in this context is the comparison of investment alternatives by comparing the magnitude of performance indicators. The resolution of detailed models can be reduced in order to decrease the computational requirements and to enable a higher number of simulation runs.

Tactical Tactical decisions – such as the purchase of an additional machine or the use of a new active material for electrodes – require more accurate results for a sound evaluation of the effects on other system elements. The simulated period of time may be shortened with reference to the specific planning task. For example, if an additional machine shall increase the output it may be sufficient to compare scenarios for the weekly or monthly output.

Fig. 4.33 Characteristics of simulation models for strategic, tactical, and operational planning regarding accuracy, resolution and precision of simulation and considered time scale



Operational Operational decisions – such as scheduling of certain jobs – refer to short term decisions which can be based on a large amount of available data and requires high accuracy. Models must be very accurate and of high resolution to allow the valid comparison of very similar decision options considering a limited time period (e.g. a shift or a week).

Figure 4.33 illustrates the described characteristics of simulation models regarding accuracy and considered time scale for different planning perspectives.

Moreover, different stakeholders may have different weighting of individual objectives. Consequently, it is relevant to clarify the specific objectives of the simulation to determine the required models and their necessary model resolution.

4.7.3 Definition of Required Models (III)

The framework (Fig. 4.5) illustrates the model classes of a multiscale simulation of battery production systems. However, the integration of several detailed models into a simulation increases the complexity of the overall model. That means, that increased functionality and enhanced possible results are achieved at the cost of higher modeling effort, a higher error rate (e.g. due to rounding), and the risk of reduced acceptance of the results. Consequently, it has to be aimed for the balance between high model complexity and result accuracy. It has to be examined which models are needed to generate results in the resolution needed for the evaluation of the defined objectives. For this purpose, it is necessary to collect information about all production system elements within the system boundaries and to identify relevant specifications such as operational times and energy data³⁸ of machines or TBS systems. This forms the foundation for the definition of required models.

In any case, a process chain model is required for simulating the material flow and coordination for all other models. In addition, machines and other systems have to be included in the multiscale simulation if they

- are part of the process chain,

³⁸Energy demand related data can be acquired from machine specification of manufacturers documentation. If detailed data are required, data acquisition can be used to measure the actual power demand. Strategies for selecting suitable types of acquisition are discussed in Thiede et al. (2013a).

- have high energy or power demands, or
- have influence on product characteristics through related processes.

If a machine or system meets one of these criteria, it can be modeled in different levels of detail. Two main model types can be distinguished:

- simplified state-based model (such as the proposed generic machine model), or
- detailed component based, state-based, empirical, or physical model.

If a machine is part of the process chain, its behavior has to be modeled at least in terms of operational states. This is needed by control strategies of process chains to determine the routing of processing units. Furthermore, if a machine or system has a high energy demand, it is important to include a model which determines the power demand even if the machine is not part of the process chain. A suitable method for assessing the relevant machines or systems regarding energy demand is an energy portfolio which clusters all machines/system with respect to power demand and operational time per time period (Posselt 2016). This method is also suggested by Thiede (2012) for selecting relevant machines/systems which should be considered in simulation studies. If a machine or system has high or moderate (nominal) power demand and a high or moderate operational time or utilization factor, it should be included in the simulation.³⁹ However, this method does not consider the volatility of the power demand. If the demand is rather constant for each operational state, a generic state-based model is sufficient to simulate the power demand profile. If the power demand is very volatile, detailed modeling of the machine/system and its components may be favorable in order to increase the result accuracy. Thus, a second portfolio is suggested to cluster machines/systems regarding power demand and its volatility. Figure 4.34 shows both portfolios. The determination of the volatility and the definition of the boundary between high and low volatility depend on the required accuracy of the simulated energy demand (see Step II). As one feasible approach, it is suggested to analyze the power demand values of a machine regarding a measure of variance. However, it is important to consider the variation in power demand in relation to the processing time of a machine. If the power demand fluctuates by a high magnitude (e.g. periodically) within intervals of only a few seconds, but the operational time of a machine is a couple of hours, the energy demand of the machine may be rather constant.⁴⁰

If a machine additionally has noticeable effects on the associated process – and consequently on the product characteristics – it should be modeled in the required level of detail for considering the impacts on the processing results. Examples of effects are machining tolerances, tool wear, or random deviations. Figure 4.35 summarizes the selection of production system elements and the allocation of a suitable modeling type.

³⁹If it is not clear how often and for how long a machine/system is used, it is possible to perform simulation runs with generic machine models to determine the operational times of machines/systems for the given production system.

⁴⁰In this case, filtering or smoothing of the power demand profile with adequate filtering parameter for the interval length allows to generate better insight in the relevant deviation.

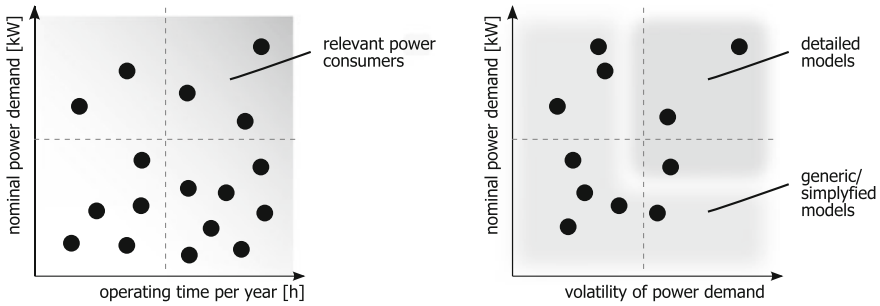


Fig. 4.34 Portfolios for selection of energy demanding systems (*left*) and allocation of model type (*right*)

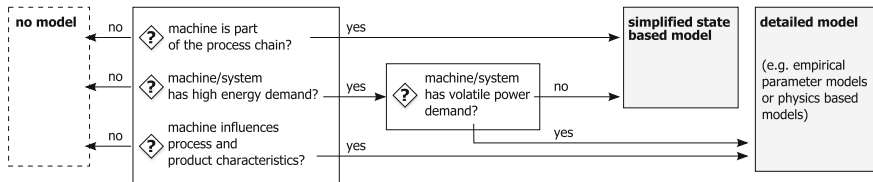


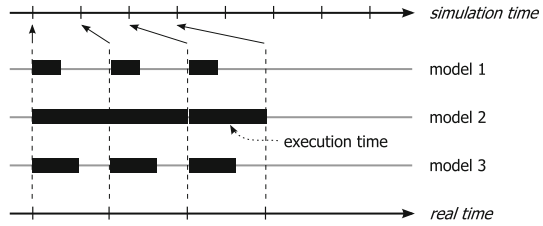
Fig. 4.35 Decision tree for selection of model types for machine models

If desired, the evaluation of product characteristics requires the modeling of processes and their impacts on product characteristics as well as a product model to store the results. Some processes could be modeled based on physical equations. If no knowledge about theoretical relations exist, empirical data from experiments may allow to derive relations between process parameters, environmental conditions and resulting product characteristics.

4.7.4 Modeling, Implementation (IV), and Coupling of Models (V)

It is necessary to develop a concept for each required model which defines the model logic and specific outputs based on the intended results. For this purpose, each real world system or process which has to be modeled must be analyzed to derive a concept model. Since a model has to be precise enough to achieve the defined objectives, a fundamental understanding of the system or process is needed to decide which essential characteristics should be considered in the model and which are negligible. Subsequently, the concept model is specified and transferred to a formal model (e.g. based on equations, state charts, etc.) and finally implemented in an executable software model (Wenzel et al. 2008).

Fig. 4.36 Data exchange between models at different simulation time steps



The selection of a software tool for a specific model depends on various factors. It may be best to select the most suitable tool for each specific model. For example, a DE simulation tool is suitable for the simulation of a process chain while tools for continuous models (DS) are required to realistically imitate a compressed air system or the thermal building ambient conditions over time. Furthermore, it may be reasonable to choose simulation tools based on their ability to share information with other models. However, it may also be adequate to use software which is already available or intended to be used for other models of the multiscale simulation. Wenzel et al. (2008) provided a checklist for model implementation.

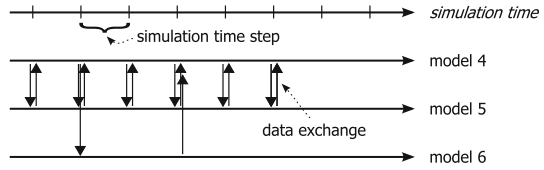
Executable simulation models have to be connected within the multiscale simulation. Since there are no established methods, guidelines, or suggestions for selecting the most suitable coupling concept for specific model couples, it is suggested to consider the following criteria.

One criteria is the timing of data exchange between models since different models may require information at different points of time and with different accuracy. For example, while it might be sufficient for some variables to be sampled and communicated at distinctive time steps, it might be necessary for other variables to communicate the integral or regression between two time steps. Furthermore, some models run during the entire simulation while other models only provide results at distinctive time steps. For example, static parametric models may provide results if requested at single events while continuous models provide values at each time step. Figure 4.36 illustrates these different forms of data exchange. It implies that some models can be executed sequentially (e.g. machine and process models within a linear process chain) while other models have to run continuously in parallel (e.g. models for HVAC systems and the building). The utilization of a middleware is reasonable if models running in parallel have to exchange data during simulation.⁴¹

Another criteria is the execution time (in particular of one iteration). Some models may have a very long execution time due to the amount of required calculations even if the simulated time period is relatively short. Examples are detailed DEM or FEM simulations. If such models would be connected to a process chain model, the latter would have to wait until slower models provide results. Figure 4.37 illustrates the

⁴¹The advantages and disadvantages as well as characteristics of synchronization types are discussed in various publications (e.g. serial versus parallel (Sweafford and Yoon 2013) or strong versus loose coupling algorithms such as Jacobian-based simulation algorithms (Sicklinger et al. 2014). The effects of smoothing and extrapolation of exchanged values is studied by Kossel (2011).

Fig. 4.37 Effect of different execution times of models



effect of different execution times in real time with respect to the simulation time steps. The coupling of models via a middleware would allow to provide information about the progress of detailed models to the process chain model so that other parallel events could already be started. Alternatively, time intensive models may be substituted with simplified mathematical or parametric models. This could drastically reduce the run-time making the model usable in a coupled simulation (Brecher et al. 2009).

Several recommendations were derived from the discussed criteria. If a middleware software and interfaces to all used software tools are available, the middleware concept is suitable for all models. Another suggestions is that if all models are available in the same software tool, model integration is a reasonable concept (Thiede et al. 2016). In any other case, each model combination has to be examined also regarding the following recommendations summarized in Table 4.4.

Table 4.4 Recommendations for model coupling

Characteristics of model couples	Offline coupling	Model integration	Direct coupling	Middleware synchronization
Parallelism of several models with different time scales	○	●	●	●
Interactions between models during model execution	○	●	●	●
High ratio between execution time (of each iteration) and model (simulation) time	◐	○	○	●
High number of models to be coupled	◐	○	◐	●
Models available in the same software environment	◐	●	○	○
Only two or few models, available in specialized software	●	○	●	◐

●: recommended; ○: not recommended; ◐: reasonable, depending on circumstances

4.7.5 *Verification and Validation (VI)*

Each specialized model and the connected multiscale model have to be verified and validated (VDI 2014). Verification means, that an implemented model is tested regarding providing the correct results based on the intended model logic without errors. Validation means, that a model is tested regarding representing the corresponding real world system precisely enough with respect to the defined simulation objective. For the validation of the connected multiscale model, a focus has to be set on the validation of cause-effect relations between different production system elements. In general, verification and validation can both be supported by various methods and techniques. Examples are validation based on historical data, fixed or extreme value tests, sensitivity analysis, and sub model tests. Further procedures for verification and validation as well as common methods and techniques are presented for example by Rabe et al. (2008) and Wenzel et al. (2008).

4.7.6 *Definition (VII) and Execution (VIII) of Simulation Runs*

Simulation runs have to be defined (step VII) by creating consistent parameter sets and boundary conditions such as simulation time periods and seed values for random number generators.⁴² The definition of simulation runs has to be aligned with the simulation objectives (from step II). Simulation runs represent different production system scenarios which should be compared. Examples are the evaluations of impacts resulting from different processing times, energy demands, shift times, facility locations, or used raw materials on all of the defined performance indicators. If the impacts of specific parameters shall be analyzed in detail, multiple simulation runs can be defined in order to generate results for a sensitivity analysis. In this case, only specific parameters are changed while all other parameters are kept constant. If stochastic variables are included within the simulation, it is also important to conduct multiple simulation runs for the same scenario in order to increase the quality of the results (Wenzel et al. 2008). However, there is no established rule for the definition of the required number of simulation runs and it is often based on experience (März et al. 2011). Kelton (2000) suggested to use traditional experimental design methods to defined simulation experiments and to derive the best combination of input parameters.

After the definition of simulation runs, the multiscale simulation model is used to execute these simulation runs and to generate and prepare the resulting data for the following evaluation (step VIII). Depending on the execution time of the overall

⁴²Using a fixed seed value means, that stochastic variables (e.g. for machine failure) are determined based on a random number generator but that these determined values are the same for each simulation run. This allows to compare different simulation runs with stochastic variables. If random seed values are used, the stochastic variables are different for each simulation run.

model, this step may require a lot of time. The results have to be stored in data formats (e.g. spread sheets) which are easily accessible for evaluation even when simulation tools are terminated.

4.7.7 Evaluation of Simulation Results (IX) and Objectives (X)

The first evaluation (step IX) refers to the analysis of the quality of simulation results. It has to be checked if the results are valid and plausible. Moreover, it has to be checked whether they are suitable for the evaluation of the simulation objectives or if required results are missing or if the resolution of results is not high enough. Furthermore, if the results indicate hot-spots within the simulated production activity (e.g. bottle necks or machines with very high energy demands), it has to be checked if these relevant aspects are covered by the results precisely enough or if more detailed models are required for a deeper analysis. In the latter case, models have to be modified or additional models have to be created.

The second evaluation (step X) refers to the analysis of the simulation objectives based on the simulation results. The performance indicator values – based on the definition in Table 4.3 – resulting from different simulation runs have to be compared to derive insight into the system behavior and to evaluate the benefits and shortcomings of the scenarios. This step requires strong involvement of experts from different disciplines. If the results are not sufficient for the evaluation of the defined objectives (e.g. the simulated time period is not long enough), additional simulation runs have to be defined and executed.

4.7.8 Reporting of Evaluation Results (XI)

The quantitative and qualitative findings from the result evaluation have to be combined within a report which addresses the defined objectives. The results will be used by planners from the involved disciplines to derive recommendations for real world decisions towards the improvement of a battery production system. Reports have to contain a description about the utilized simulation models, the characteristics of simulation runs, performance indicator values for each simulation runs, as well as a summary of the results and derived conclusions about the scenarios. A report has to state the impacts on production costs, environmental impacts, and quality of batteries or battery components. Value stream maps can be used for each produced product type (electrodes, cells, modules, systems) showing the process sequences and highlighting the most crucial processes regarding production time, energy demand, and material consumption. Specific requirements for reports have to be discussed with the involved stakeholders. Overall, it is important to clearly state and collect new findings regarding the system behavior in order to establish a knowledge base which allows deriving new improvement measures or experiments.

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Chapter 5

Implementation of a Multiscale Core Model

The concept of a multiscale simulation for battery production systems is centered around a process chain model which acts as a coordinator for other models. Such process chain model determines the activities within a production system and derives inputs for detailed models of system elements. Consequently, this model is a key component of multiscale simulations.

For this reason, an adaptable multiscale core model was developed and implemented, which can be configured to any kind of process chain, contains essential sub-models, which can be extended by external simulation models. The intention behind this model is to provide a flexible software tool which contains the minimum functionality needed for the realization of specific multiscale simulation applications. To serve this purpose, the core model allows simulating the material flow of processing units and contains generic models for machines, product characteristics and processes, lighting, and workers. Furthermore, the model has interfaces for connecting external simulation models such as detailed process models, TBS system models, or a building model. As an example, a model for a compressed air generation system was implemented which is connected to the core model via a middleware software. This chapter presents the architecture of the core model (Sect. 5.1), its components (Sect. 5.2), the compressed air generation system model (Sect. 5.3), the synchronization concept for the connection of external models (Sect. 5.4), as well as the verification of the overall model (Sect. 5.5).

5.1 Core Model Architecture

The model architecture describes the components and their interactions within the core model. The main function of the core model is the simulation of the flow of

processing units through a virtual shop floor consisting of different machines¹. Processing units are of a certain product type which specifies the sequence of required production steps, each of which is allocated to one or several machines. Furthermore, processing units belong to jobs which are characterized by a job type and a quantity of final products. During production time, processing units search for suitable machines, move to these machines and are processed until the last production step is finished (see Sect. 4.3.2). Processing units and machines are modeled as agents with individual properties based on agent classes. This allows the replication of agents and a flexible definition of process chain layouts.

The core model also contains models for lighting and workers (agents) according to the multiscale model structure shown in Fig. 4.28. All system elements are assigned or dynamically linked to building zones. The core model aggregates all variables on the main level – and if necessary for each building zone –, provides data to interfaces for external models, and determines performance indicators. These indicators are visualized within a cockpit for result evaluation during simulation runs. The model also has an export function to make the results available after simulation. Figure 5.1 drafts the model architecture by showing the different sub-models and components with their inherent variables and information, as well as the interfaces for external models.

Based on this architecture, the core model is implemented within the software AnyLogic. AnyLogic is a hybrid simulation tool which enables combining DE, DS,

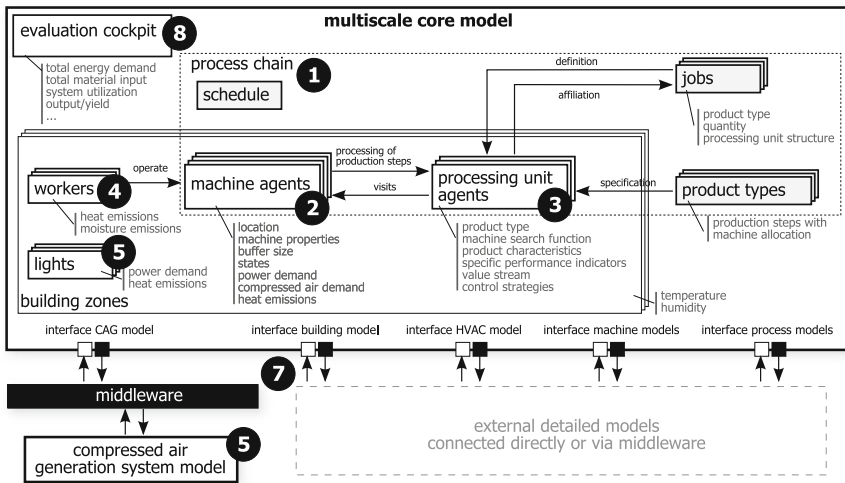


Fig. 5.1 Architecture of the multiscale core model with interfaces for external models

¹As stated in the concept derivation, machines can also be substituted by workstations which do not utilize any equipment.

AB, and SD simulation within one model. The software is based on the programming language Java.²

5.2 Core Model Components

As shown in Fig. 5.1, the main components of the core model are sub-models for jobs, product types, processing units, machine agents, workers, lights, building zones, the evaluation cockpit, and schedules. This section describes these components.

5.2.1 Jobs and Product Types

Jobs and product types are objects used for defining and controlling the sequence and routing of processing units. Jobs correspond to requests for the production of a quantity of a product type. As an example, a job is created for the production of 1000 battery cells of a certain type or for the assembly of 200 specific modules. Depending on the product type, different processing units are required to simulate the routing of a job as well as to track product characteristics along the process chain. For this reason, job objects define the type and quantity of processing units which are required to simulate the production of a desired quantity of final products.³ In the process chain model, a job is characterized by a job type, the desired quantity of final products and the associated product type(s). Three different job types have been predefined. The first is a generic job type which can be used to imitate the production of one product type in a certain quantity. This job creates a number of processing units corresponding to the desired quantity. Processing units can be treated as single product units or as batches.⁴ This allows using the generic job type if identical product units should be produced. The second job type addresses the production of battery cells. A job defines two processing units, each of which represents an electrode batch. When both batches are completed, the job defines processing units according to the desired quantity of cells. A job is completed when the last related processing unit (cell) is finished. It is necessary to specify the product types for anodes, cathodes, and cells. The third job type is usable for the combined assembly of modules and systems. The desired quantity of systems has to be specified to derive the required number of modules.⁵ As soon as enough modules are finished to complete a system, a processing unit of a system may start production. Table 5.1 summarizes the characteristics of the three job types.




²Further information about AnyLogic can be found on www.anylogic.com.

³As an example, the production of 100 cells requires two processing units representing the electrode batches and 100 processing units for representing each cell.

⁴That means that the number of processing units is different for single unit or batch production. Example: If 100 product units should be produced in batches of 20 units, required are five processing units. A generic job would have to be defined with a quantity of five.

⁵The number of modules per system has to be specified in the system's product type definition.

Table 5.1 Characterization of job types regarding quantity, product types (anodes (a), cathodes (c), cells (ce), modules (m), and systems (s)) and related processing units

Job type	Quantity (Q)	Product type (PT)	Processing units
Generic	Q	PT	
Cell	Q_{cell}	$PT_{anode}, PT_{cathode}, PT_{cell}$	
System	Q_{system}	PT_{module}, PT_{system}	

The definition of product types allows the differentiation of electrodes, cells, modules, and systems. Moreover, a product type can specify different variants of these products such as electrodes of different materials or cells with different numbers of layers. In this model, product types specify processing units regarding their production step sequences, the allocation of production steps to machines, as well as processing times and material inputs per production step.

In summary, the job and product type objects make it possible to configure the model to simulate a specific process chain. It can be used to simulate different production stages – according the defined system boundaries – separately or within a combined process chain.


5.2.2 Processing Unit Agents

Processing units are modeled as agents based on a processing unit agent class. On process chain level, processing units are displayed by simplified interactive icons which indicate the ID and product type. Moreover, a dynamic circle indicates the progress during processing. Within each agent, the icon contains further information about the current state, accumulated material cost and direct embodied energy (DEE), as well as an illustration of the current product state. Figure 5.2 shows an exemplary icon of an electrode processing unit within the first mixing process, still in raw material state.

This agent class contains a state chart for representing the states of a processing unit during production, parameters for defining the product specifications, the related job and assigned product type, variables for product characteristics, input materials, and direct embodied energy as well as an algorithm for selecting the next suitable machine. The state chart of a processing unit indicates if a processing unit is already started, searches for a next machine, moves to a machine, is at a machine, or is completed after the last production step. These states allow to control and monitor the behavior of processing units within the process chain. When a processing unit is created and initialized, it searches for the first machine. For this task, the algorithm is implemented according to the shortest throughput time control strategy.⁶ This

⁶Other control strategies and selection criteria are possible (see Sect. 4.3.2).

Fig. 5.2 Icon of an electrode processing unit (here: processing unit nr. 1 of product type 2)



visible on
upper level


New machine found?: ●

Number of states: 5

Current state: 0

Material cost [€]: 17.354

DEE [kWh]: 691.617



not visible on
upper level

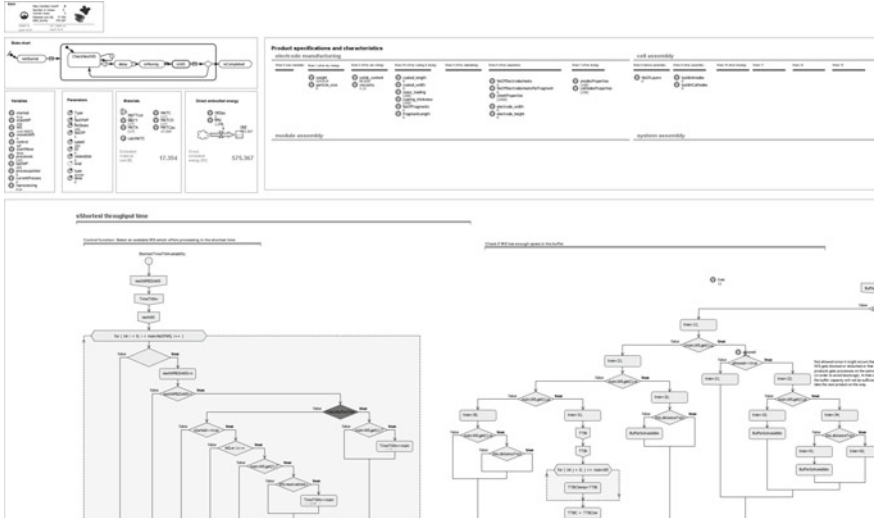


Fig. 5.3 Screenshot (for illustration only) of processing unit agent class content: *top left* icon, state chart, parameters and variables; *top right* product specification and characteristics per state; *bottom* algorithm (action chart) for machine selection

algorithm requires information from machine agents such as the location and the time until availability.⁷ After a machine is selected, the processing unit agent moves to the machine. When the processing is finished, the machine agent sends a signal to the processing unit which searches for the next machine. If no available machine can be found, the processing unit blocks the current machine. In this case, the search algorithm stays active until a machine becomes available. This logic corresponds to the processing unit flow illustrated in Fig. 4.9. Figure 5.3 presents a screenshot of the processing unit agent.

The flow of processing units is visualized by a value stream map. For each production step, the model creates a data field which is filled with related performance indicators such as processing time and waiting time. This allows analyzing if, where, and for how long a processing unit had to wait prior to processing. Also it is possible to determine the overall time of production for each processing unit. Each agent con-

⁷If external machine models are used, the remaining processing time might not be known or predetermined but a result of the simulation. In this case, the algorithm considers a very long time until availability. As a result, a machine is usually not selected unless no other machine is available.

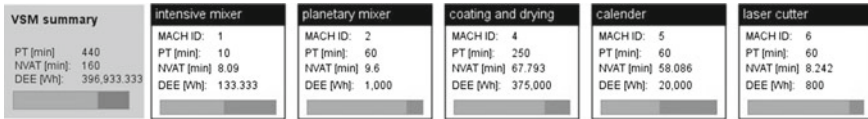


Fig. 5.4 Screenshot of an exemplary VSM representation within a processing unit agent

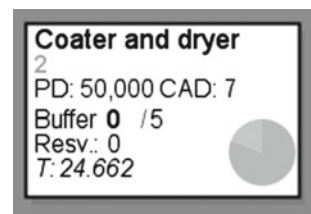
tains a VSM representation showing the history of processing. Figure 5.4 presents a screenshot of an exemplary VSM representation of an processing unit for an electrode batch. The figure shows the sequence of processes for an electrode job with related processing data as well as a summary of derived indicators such as lead time. The bars indicate the productive and non-productive time shares. Furthermore, the representation shows the direct energy demands from processing at each machine.

5.2.3 Machine Agents

Machines are also modeled as agents based on a machine agent class. On process chain level, machines are displayed by interactive icons which indicate machine name, number, current state (by the color of the border), the current demands, machine temperature, the number of processing units within the buffer, and the time shares per state. Figure 5.5 shows an exemplary screenshot of a machine icon.

The dynamic characteristics of a machine are determined decentralized within a machine agent. On the inside, each machine agent consists of a flow chart for modeling the processing unit agent flow through the machine, a state chart for modeling of possible states and their transitions, parameters for specifying machine properties (e.g. location, buffer size, etc.)⁸, and variables for describing the machine characteristics (e.g. power demand, compressed air demand, and heat emissions). Elements of the AnyLogic enterprise library are used to model the processing unit flow through a machine. These elements allow to control the routing of processing unit entities entering a machine to a buffer (queue element) which is closed (by a hold element) in case the machine is still ramping-up. After ramp-up, a processing unit is routed to the actual process (delay element) and – after the processing time – the processing unit

Fig. 5.5 Representation of a machine agent on process chain level



⁸Machine parameters can be externally configured in spreadsheets and imported to the model.

leaves the machine if a new machine (or a buffer) is available for further processing. If a processing unit does not find a next machine, the processing unit blocks the current machine. If a machine failure occurs, the state chart switches to the failure state and it is assumed that the machine behaves as in idle state. The processing of the current processing unit is resumed after the failure is resolved.⁹

The flow chart communicates with the state chart which describes possible machine states according to the definition of the generic machine model. The state chart further determines the demands for electric power and compressed air. Furthermore, the state chart allows to determine the time shares of different operational states such as ramp-up time, idle time, and processing time. This also enables to derive the utilization of each machine. The power demand is input to the calculations of machine temperature and heat emissions which also require certain machine parameters (mass, surface area, etc.) and the current building zone temperature.

In addition, machine agents contain an algorithm for determining the time until a machine is available for processing of a next processing unit. This algorithm considers various factors such as the current state and buffer level, remaining processing time, future processing times of buffered processing units, and remaining movement times of processing units which are currently moving to a machine. Figure 5.6 shows a screenshot excerpt of the machine agent class content.

Machine agents can further contain process models and a set of associated process parameters. Process models describe how a process modifies particular product characteristics of processing units. Depending on the specific process, process models can be realized by functions which calculate the resulting product characteristics based on specifications and existing characteristics of a processing unit. Alternatively, if the processing results vary over time or different sequential activities can be distinguished, it is also possible to use timed state charts to define the execution of functions in more detail.¹⁰

Finally, machine agents are responsible for the connection of external machine models. For each machine, a machine agent has to be placed within the process chain. If an external machine model is used, the machine agent coordinates the execution of the external model. For this purpose, the state chart contains a section which controls the interaction with external models. This is important since the external model has to behave according to the defined states. Thus, the state chart of the machine agent is used to send and receive coordinating signals. The machine agent also receives values for power and compressed air demand from the external model. Table 5.2 lists the variables for communication with an external model.

This set of variables may be extended for specific purposes. For example, if an external machine model simulates the detailed thermal behavior of machine compo-

⁹Different failure behavior could be implemented.

¹⁰This might be relevant for processes with long processing times. As an example, the process characteristics during coating and drying may vary over time if the machine temperature increases or the coating thickness increases due to variations in the coating device. The characteristics of the coating layer may vary over time and may differ for different fragments of the layer. In this case, a state chart may repeatedly trigger the process model function.

Fig. 5.7 Representation of a worker agent on process chain level



5.2.4 Workers

Within the core model, it is assumed that each machine needs at least one worker for operation. Workers are modeled as agents.¹¹ As soon as a processing unit has selected a machine which is currently turned off, this machine agent requests the required number of workers. On process chain level, worker agents are represented by an interactive icon, which is shown in Fig. 5.7. Each worker agent contains a state chart with the states standing, walking, light work, and hard work. During walking, a worker moves along a defined path to the target location. The current location of a worker is mapped with the building zone areas and the heat and moisture emissions are allocated to the current zone. In general, modeling of worker agents allows either to determine the minimum number of workers or if a specific number of workers if sufficient for the operation of all machines. Furthermore, it allows to determine the heat and moisture emissions to each building zone. This aspect may be relevant for dry rooms which accept only a certain internal moisture intake.

5.2.5 Building Zones and Lighting

The core model allows defining building zones within the global shop floor coordinate system. Zones are characterized by area, temperature, lighting condition, and inside heat and moisture emissions. Heat emissions are caused by machines, workers, and lighting. For this reason, machines are assigned to building zones according to their position within the shop floor and processing units and workers are linked to zones based on their current location. The core model aggregates these emissions for each building zone and provides the internal loads to an interface for the connection of a building model. In return, a building model is expected to provide the inside temperature – and, depending on the specific building model – humidity of each zone. For this purpose, the definition of building zones in the process chain model has to match the zone definition in the external building model.

Each building zone has light sources which can be operated according to different schedules and control strategies. In the current model, the lights are turned on when a worker enters a zone and turned off if the last worker leaves a zone.¹² The control of lighting for each zone is realized by a state chart which assigns a state-based power

¹¹The model contains a pool of workers which are all able to operate any type of machine. It would also be possible to specify the skills and characteristics of each worker agent in more detail.

¹²It is assumed that all lights within a zone are turned on and off simultaneously.

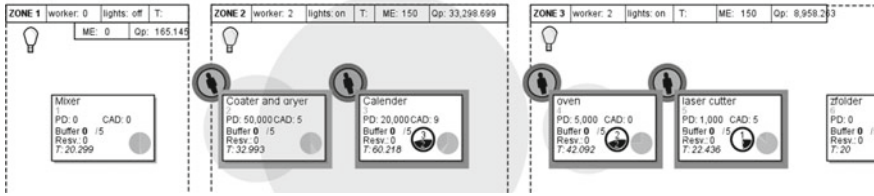


Fig. 5.8 Screenshot of core model level with zones, machines, workers, and processing units

demand for lighting. This power demand depends on the required lighting intensity, efficiency, zone area, and type of light source. The power demand equals the heat emission to the building zone. Figure 5.8 presents a partial screenshot of the process chain level showing multiple machines and workers within three building zones. The characterizing variables of each zone are presented at the top of each zone. The circles around machines indicate the current intensity of heat emissions.

5.2.6 Shift Schedules

Mostly, production facilities operate only during defined shift hours according to schedules. Considering these schedules in the simulation is important since machines and lights may be turned off and HVAC operation switched into energy saving mode during non-operation hours. Furthermore, the output of final products per time period strongly depends on the shift schedules. AnyLogic allows simulating dates and times based on a calendar. This enables defining schedules and deriving control signals for machines, TBS, and machine operators. In the implemented model, it is required to define a daily start time and a shift duration. However, it is also possible to define other schedules considering breaks and weekends.

5.2.7 Evaluation and Visualization

Simulation runs generate various data and values for defined performance indicators. The AnyLogic model allows browsing through all agents and model components to inspect specific variables, plots, and charts. Furthermore, on core model level, the evaluation cockpit provides an overview about the key indicators of each simulation run and allows to visualize and export time series of indicators. Plotting various system variables over a longer period of time enables the analysis of effects acting on a larger time scale such as weather impacts. Also it supports the observation of the required initiation time or so-called warm-up period of the simulation

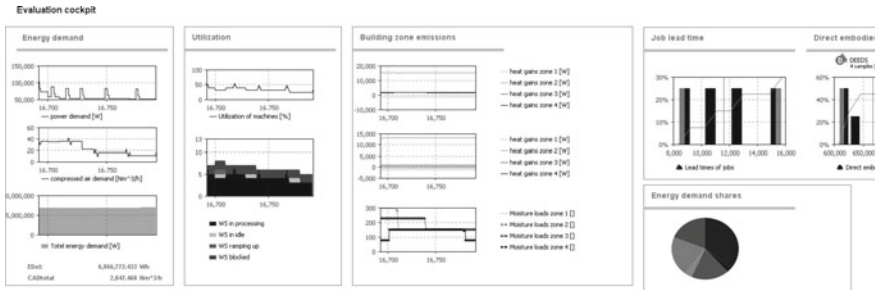


Fig. 5.9 Screenshot (for illustration only) of the visualization of performance indicators within the model cockpit (energy demands, process chain utilization, building zone characteristics, lead times per job, time shares of machine operation, etc.)

model.¹³ Examples of indicators in the cockpit are the electrical power demand of all machines, the compressed air demand of all machines and the resulting compressor power demand, the process chain utilization, as well as the aggregated heat and moisture emissions per building zone. In addition, a pie chart illustrates the shares of demanding systems on the overall energy demand. Furthermore, the cockpit contains histograms of the lead times and embodied energy of jobs as well as a display showing the current output of final products. Figure 5.9 shows a screenshot of the evaluation cockpit.

5.3 Compressed Air Generation System

The model for a compressed air generation system is implemented in the software Matlab Simulink based on the previously described concept model. The model consists of the three blocks tank, controller, and compressors. The tank block contains the functions for the calculation of the system pressure *cap*. Inputs to the block are the compressed air demand from the process chain, pressure losses due to leaks, and the air supply from the compressor. The output of the block is the system pressure which is an input to the controller block. The controller determines the air supply required to maintain a system pressure within the accepted interval. It generates signals for switching the compressor on and off. In the compressor block, Stateflow elements are used to model the compressor states off, on, and idle as well as to determine the air supply, the state-based power demand and the count of switching cycles. Figure 5.10 shows a screenshot of the implemented model.

¹³The warm-up period refers to the time from the start of a simulation run until the model represents the normal or balanced behavior of the real system. For example, in the simulation of a series production, the model is warmed-up if all machines are operating and buffers are filled. This period has to be considered in the result evaluation.

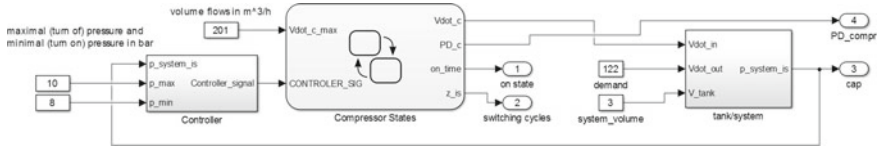
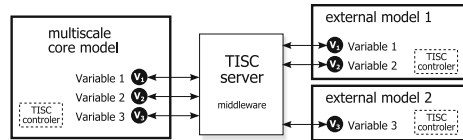


Fig. 5.10 Screenshot of compressed air generation system model in Simulink

Fig. 5.11 Exemplary structure for model coupling via TISC middleware



5.4 Coupling and Synchronization of Models

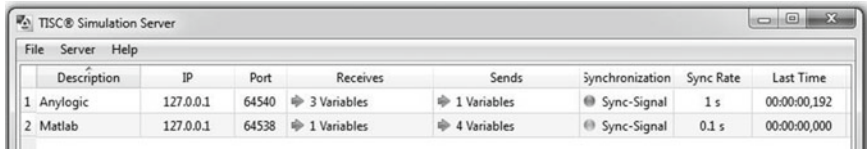
The core model provides two different types of interfaces for the coupling of external models. First, static numeric models can be connected by a direct interface.¹⁴ The process chain model calls the external model and waits for the results of the external model in order to continue the simulation based on these results. For example, this interface can be used to utilize static process models which calculate resulting product characteristics based on empirical data samples. Such model can be called by a machine agent during the processing state.

Second, external simulation models can be coupled with the core model by using a middleware software. The TISC software suite is used which provides different packages for establishing co-simulations.¹⁵ The core element is the TISC Center which connects different client models. The TISC Center is responsible for the co-simulation configuration, synchronization, and data exchange between all models.¹⁶ Figure 5.11 illustrates the connection of external models to the core model using TISC. At model start-up, AnyLogic has to load the required Java classes and connect to the TISC server. Moreover, all exchanged variables have to be defined at model start up. In the AnyLogic model, a reoccurring event triggers the synchronization by sending values to the TISC server, waiting for a synchronization signal, and writing the received values to the corresponding variables in AnyLogic. Figure 5.12 shows a screenshot of the TISC server control window.

¹⁴This coupling approach was used in Schönemann et al. (2016).

¹⁵TISC is offered by TLK-Thermo GmbH. Information can be found on www.tlk-thermo.com.

¹⁶The TISC suite provides interfaces to various software tools such as Matlab, Modelica (Dymola), Ansys, and others. However, TISC did not provide a standardized interface for AnyLogic. For this reason, the TLK-Thermo GmbH developed a TISC-to-java interface which enables AnyLogic to communicate with TISC via defined Java classes. This support is gratefully acknowledged!



Description	IP	Port	Receives	Sends	Synchronization	Sync Rate	Last Time
1 Anylogic	127.0.0.1	64540	3 Variables	1 Variables	Sync-Signal	1 s	00:00:00,192
2 Matlab	127.0.0.1	64538	1 Variables	4 Variables	Sync-Signal	0.1 s	00:00:00,000

Fig. 5.12 Screenshot of the TISC server control window

5.5 Verification

The multiscale core model was verified during implementation. To demonstrate the used verification procedure, a generic job and model configurations were defined which support testing of all model functions and generating transparent results which are comparable with static calculations. The job defines the production of one batch of a product type. The product type requires three production steps, each of which is allocated to one machine and needs 60 min of processing time. The three machines are located in two different building zones both with an installed lighting power of 1500 W. Table 5.3 lists the characteristics of the machines.

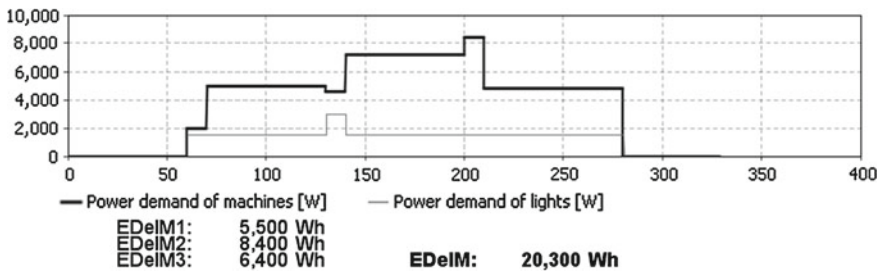
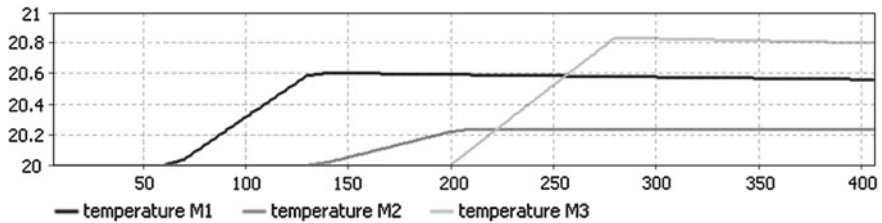
The energy demand per machine can be calculated based on the time shares for each operational state and the associated power demands. The results of static calculations state that the energy demands of the machines for the production of one batch are 5,500 kWh for machine 1, 8,400 Wh for machine 2, and 6,400 Wh for machine 3.¹⁷ Figure 5.13 presents a plot of the resulting power demand profile and the values of the resulting electrical energy demands. The figure also shows the power demand of lighting. During the operation of the first machine, the lighting in zone 1 is turned on. Afterwards, the lighting in zone 2 is turned on. Since machine 1 is in idle mode for 10 min after processing, there has to be a short period in which the lighting in both zones is turned on. This behavior can be seen in Fig. 5.13. Moreover, the power demand profile allows verifying the correct order of production steps. And since the lighting is turned on and off by workers, the power demand profile of lighting allows to conclude that workers enter and leave the zones correctly.

Similarly, in order to verify the determination of the machine temperature, the simulation results are compared to static calculations. The temperature of a machine can be calculated by using the equation $Q = m \cdot c \cdot \Delta T$. With the values for the mass and specific heat capacity, the power inputs, and an initial temperature of 20 °C for each machine, the resulting temperatures of the three machines can be calculated to be 20.61, 20.23, and 20.84 °C. During simulation, the model determines the increase of the temperatures up to the expected values, as shown in Fig. 5.14. After the power is switched off, the machines cool down due to the colder surrounding environment. The calculations of heat emissions of machines, workers, and lights as well as their allocation to building zones were also verified.

¹⁷For example, the calculation for machine 1 is $ED_{MACH_1} = 10/60 \text{ h} \cdot 2,000 \text{ W} + 1 \text{ h} \cdot 5,000 \text{ W} + 10/60 \text{ h} \cdot 1000 \text{ Wh} = 5,500 \text{ Wh}$.

Table 5.3 Machine configuration for model verification

	Machine 1	Machine 2	Machine 3
Zone	1	2	2
$t_{ramp-up}$ (min)	10	10	10
$t_{shutdown}$ (min)	10	10	10
PD_{rampup} (W)	2,000	3,600	4,800
PD_{idle} (W)	1,000	3,600	4,800
$PD_{processing}$ (W)	5,000	7,200	4,800
CAD_{idle} (m^3/h)	0	0	0
$CAD_{processing}$ (m^3/h)	122	10	10
Mass (kg)	5,000	11,000	3,000
Spec. heat capacity ($kJ/(kg \cdot K)$)	0.6	0.9	0.7

**Fig. 5.13** Simulated power demand of the three machines and lighting**Fig. 5.14** Temperatures of the three machines

The compressed air system model was verified with an approach similar to Thiede (2012), who used a calculation example shown by Bierbaum and Hütter (2004) to verify his compressed air module. They assumed a constant compressed air demand of $122 \text{ m}^3/h$, a system volume of 3 m^3 , as well as a compressor with a maximal volume flow of $201 \text{ m}^3/h$, 30 kW power demand during operation and 10 kW during idle. Furthermore, Thiede assumed an initial pressure of 8 bars and that the compressor stays in idle mode for 60 s before being switched off. He simulated a period of one hour and the results showed eight compressor cycles and a power demand of 19.4 kWh . This scenario was also used for the verification of the developed Simulink

Fig. 5.15 Plots of compressed air demand (top), system pressure (middle), and compressor power demand (bottom)

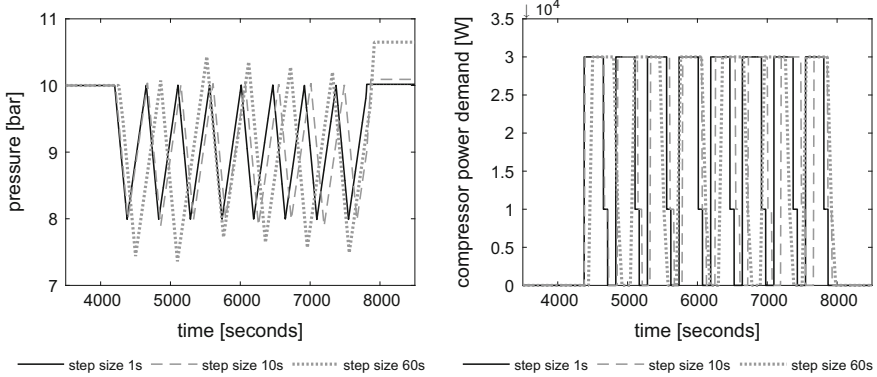
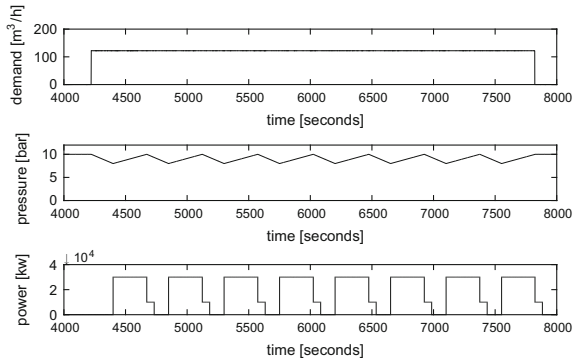


Fig. 5.16 Plots of pressure (left) and compressor power demand (right) for different simulation time step sizes (1, 10, 60s)

model. One of the machines was specified with a compressed air demand of 122 m³/h. The model generated the same results with eight cycles and 19.55 kWh.¹⁸ Figure 5.15 shows plots of the compressed air demand of the machine, the system pressure, and the resulting compressor power demand.

Another important aspect is the simulation step size of the compressed air system model as well as the step size for synchronization with the core model. In general, shorter time steps result in more accurate results but correspond to a longer execution time. The definition of the step size may have significant impact on the results. As an example for verification, three different step sizes of the compressed air system model have been tested. The results – shown in Fig. 5.16 – reveal that the step size effects the simulated system pressure and compressor power demand. If the simulation step size is larger, the lower and upper pressure limit is detected too late. This caused the compressor to start and stop the air supply too late which also effects

¹⁸The slight deviation is caused by the initial pressure of 10 bars and by the fact that the last compressor cycle was completely simulated and not stopped after exactly 3600 s.

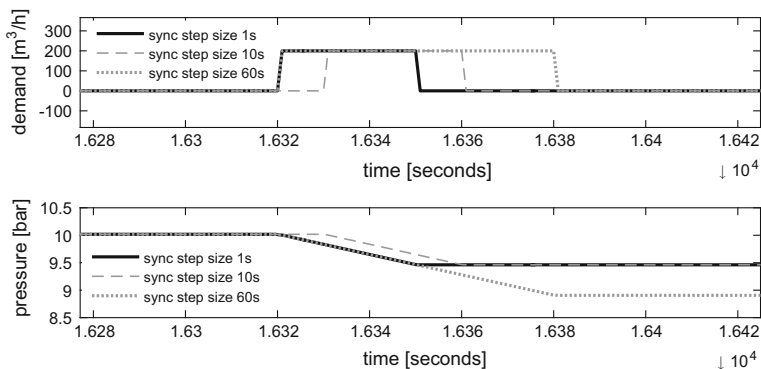


Fig. 5.17 Plots of demand (*top*) and pressure (*bottom*) for different synchronization time steps (1, 10, 60 s)

the resulting power demand of the compressor. The values for the power demand are 19.55, 19.583, and 19.50 kW for a model step size 1, 10, and 60 s respectively. Although these variations are rather low, they could add up to a larger error over the simulation period.¹⁹

In addition to the simulation step size, the synchronization step size is another relevant factor. This step size indicates how often variables are synchronized between the two models. At every synchronization step, the core model provides the current compressed air demand to the compressed air system model. That means that peaks in the compressed air demand which occur between two synchronization steps will not be communicated. To demonstrate this effect, a compressed air demand peak of 200 m³/h was generated for 30 s. Three simulation runs were conducted with synchronization step size of 1, 10, and 60 s. Figure 5.17 shows the results. It can be seen that the time of occurrence and the duration of the peak are detected wrongly for synchronization step sizes of 10 and 60 s.²⁰ This leads to the incorrect simulation of the system pressure. Since short synchronization time steps may result in longer simulation execution times, this experiment has shown that the step size must be defined according to the desired accuracy.

In summary, all relevant model functions were verified and found to provide accurate results. This includes also the correct creation of value stream maps for processing units and the functionality to use process models for the modification of product characteristics within processing units. Consequently, the model can be used as a core model for multiscale simulations. However, the exemplary results of the experiments with different model and synchronization step sizes show that it is of

¹⁹The simulation runs have been repeated for the production of 50 instead of one product unit. Shift schedules have been ignored. With a model time step of 1 s, the energy demand was 974.417 kWh. For 10 s it was 976.78 kWh and for 60 s it was 962.67 kWh.

²⁰In this example, the demand started exactly simultaneously to the synchronization step of 60 s. If it would have started just a bit later, it would have been ignored completely.

importance to set time steps which are suitable for the specific machine behavior, desired result accuracy, and acceptable simulation execution time. Otherwise, even a verified model may deliver inaccurate results.

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Chapter 6

Exemplary Application

The developed multiscale simulation concept is exemplary applied to two different battery production systems. The purpose of this application is demonstrating the use of the simulation concept, the core model, the development of detailed models, as well as the interpretation of simulation results. Since the simulation is applicable for all production stages and different objectives, the application is demonstrated for cell production (Sect. 6.1) as well as for the assembly of battery modules (Sect. 6.2).

6.1 Simulation of Cell Production

In the first study, a simulation model was created for the production of LIB cells at the Battery LabFactory Braunschweig (BLB). The twelve-step application procedure for multiscale simulations structures the following subsections.

6.1.1 *Problem Formulation (I) and Objective Definition (II)*

The BLB is a battery cell research facility.¹ It serves as a platform for interdisciplinary research on the process chain for electrodes and cells. Research fields are cell design, process improvement, sustainable manufacturing, battery cell and production system simulation, as well as data acquisition and knowledge discovery in production. The BLB is equipped with state-of-the-art production equipment such as different types of

¹The BLB was established in 2013 at the Technische Universität Braunschweig as an institution of the Automotive Research Centre Niedersachsen (NFF); www.tu-braunschweig.de/blb.

mixers, a continuous coating and drying machine, a calender, a laser cutter, automated machines for cell assembly, and cycling automates. The assembly of cells at the BLB is located inside a 150 m² dry room and is characterized by small batch sizes and manual handling operations.

The objective of the simulation is imitating the operation of the BLB – under the assumption that it operates at full capacity – and to demonstrate the capabilities of the proposed multiscale simulation approach. The simulation shall determine performance indicators such as the output of cells per time period and the utilization of equipment, as well as energy demands for different scenarios. More specifically, the simulation shall enable the evaluation of the impacts of machine configurations, processing times as well as different materials on the energy demand. In addition, the simulation shall allocate the energy demands to produced cells and create transparency about the pattern of energy demands in order to identify the most relevant machines and systems. The goal was to demonstrate the interaction of different models as well as possible results and use cases of the multiscale simulation.

6.1.2 Definition of Required Models (III)

The multiscale core model was used to simulate the material flow and to determine the operation and demands of machines. This allows the coordination of detailed models. In order to configure the core model and to define the required machine agents, machines and peripheral equipment have been analyzed. According to the proposed decision tree for model type selection, the machines of the process chain must be included in the simulation. Detailed modeling of machines or equipment may be reasonable if the energy demand is high and volatile see (Sect. 4.7.3). Hence, machines and equipment were observed regarding power demands and operational time to derive the required type of modeling for each equipment. The results of a portfolio analysis provided by Posselt (2016) were used as a starting point for the identification of machines/systems with high energy demands. In addition, an analysis of measured load profiles of machines and equipment was carried out to gather detailed insight into demand patterns. As a result, the following machines and systems have been identified to have high energy demands:

- continuous coating and drying machine
- calender
- cycling automate
- extruder
- ventilation units incl. heating and cooling
- dry room units
- chiller

These machines and systems were further investigated to determine whether the power demands are volatile and require detailed modeling or if generic models provide sufficient accuracy. As an example, the power demand of the calender was

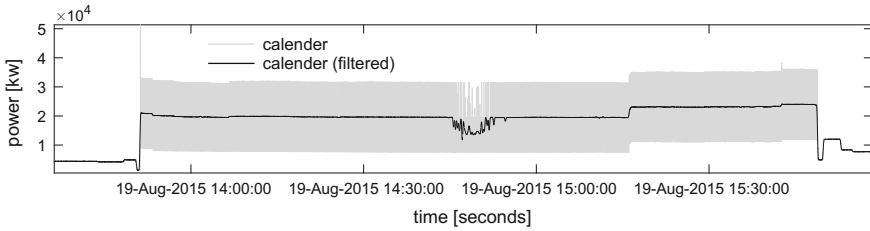


Fig. 6.1 Power measurement of calender. Unfiltered and filtered data

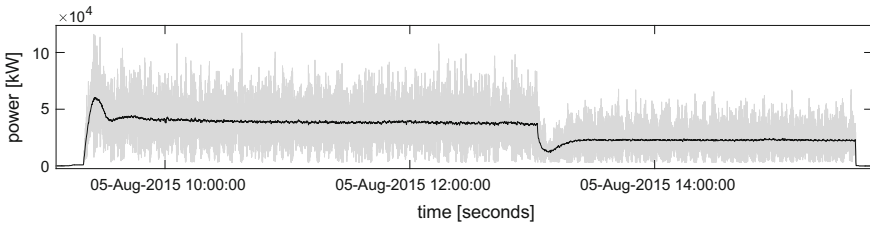


Fig. 6.2 Power measurement of coating and drying machine. Unfiltered and filtered data

examined and the power demand profile – presented in Fig. 6.1 – shows rather constant power demands for idling and processing. Generic modeling seems reasonable.

As another example, Fig. 6.2 shows a characteristic power demand profile of the coating and drying machine. During ramp-up, the power demand increases until the desired drying temperature is reached. The power demand remains constant during processing and drops to a lower level at which it stays constant again. This allows to conclude that the power demand during processing depends on process parameters. Overall, the power demand of the coating and drying machine could be simplified modeled by a generic machine model in which the state-based power demand depends on process parameters. However, if NMP solvent is used in the electrode slurry, this solvent is emitted in the drying process and the exhaust air has to be filtered before it leaves the building. A treatment system is required which consists of components with high power demands. It has to be modeled and connected to the dryer model in order to simulate the effects of different solvents on the energy demand.

This analysis approach was used for all other machines and equipment with high energy demands. It revealed that all selected machines can be sufficiently modeled with generic models due to constant power demand profiles. There are also machines with higher variation in power demand such as the z-folder or the laser cutter. However, their overall power demand is relatively low which means that a state-based modeling approach with average values is reasonable for a first estimation of the production systems energy demand. Detailed models of these machines may still be reasonable if it is desired to simulate the impacts of machine behavior on process results. For example, the speed of a gripper in the z-folder may effect the positioning accuracy of electrodes. To investigate these effects, a detailed machine model of the

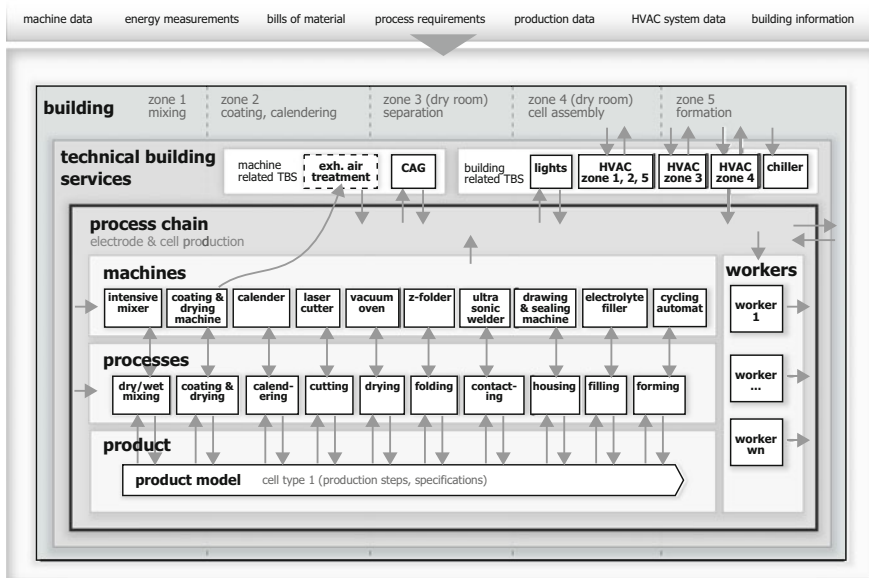


Fig. 6.3 Framework for the multiscale simulation of the BLB

z-folder with each component was created in the software Simulink with defined variables for the connection to the core model. However, these aspects and the model were neglected.

The defined models and their relations must be clearly structured within the context of the multiscale simulation. This can be realized by using the suggested framework for multiscale simulation. Figure 6.3 presents the adapted framework for the simulation of the BLB.

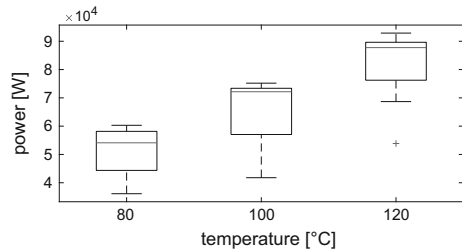
6.1.3 Modeling, Implementation (IV), and Coupling of Models (V)

The defined models have to be further specified and implemented in software. The core model, the compressed air system model, and the machine models have to be configured. In addition, detailed models have to be created for the HVAC systems including the dry room and a model for the building zones.

Multiscale Core Model

The multiscale core model was configured to represent the BLB. This required the definition of product types, material flows, jobs, machines, and building zones. An image of the building ground plan was placed in the background of the models main level and zones were defined based on the actual building zones. The machine

Fig. 6.5 Power demands of continuous coating and drying machine for three different drying temperature settings



The control strategy of the process chain had to be adjusted to account for aspects of the small scale production. It is assumed that production activity starts at 7 am and stops at 8 pm on each day (including weekends). The cycling automate is the only machine running at night. All other machines start processing only if the processing time is shorter than the remaining shift time. Furthermore, the mixing process only starts if the slurry can be used for coating at the same day. The buffer capacities at each machine are set high in order to avoid blocking. Mixers and the coating and drying machine have small buffers since they have to be immediately available at the beginning of a job.

Since battery production is highly automated, the influences of worker performance on product quality were neglected within this study.³

Building and HVAC Model

The BLB has five building zones. Zone 1 contains the mixing processes and is ventilated, heated, and cooled. Zone 2 contains the coating and drying machine and the calender. It is ventilated and heated. Zone 3 and 4 are dry rooms for cell assembly. Zone 5 contains the cycling automate and is ventilated and heated.

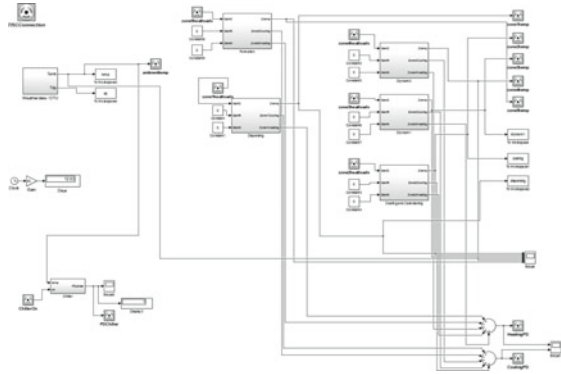
For simulation of the building inside conditions, a simplified five room model was built in Simulink using the International building physics toolbox (IBPT).⁴ Each zone was composed using construction objects for walls, windows, ceilings, as well as ventilation and air conditioning systems. Weather data were prepared based on TRY-files for Germany (DWD 2016). Figure 6.6 shows a screenshot of the building zone model. In the model, each building zone is ventilated with a constant air change rate and power demands for ventilation are assumed to be constant within each of the states operation and standby according to measurements taken at the BLB.⁵ The heating energy is supplied to the BLB as district heat. In addition to the supplied heat, the process chain model determines heat emissions of machines, lighting, and

³It is possible to implement existing worker performance models (e.g. from Baines et al. 2004) into a multiscale simulation if the results are expected to be beneficial.

⁴The open-source toolbox was developed by the Building Physics research group of the Chalmers University of Technology in Gothenburg, Sweden and the Department of Civil Engineering from Technical University of Denmark in Copenhagen. The resources and information are available on www.ibpt.org.

⁵For each zone: 8kW in operation and 5kW in standby mode.

Fig. 6.6 Five-zone building model implemented in Simulink



workers to each building zone. These heat emissions reduce the required heat supply and may demand cooling. The building model determines the resulting heating and cooling power demand required to maintain zone temperatures between 20 and 26 °C. The simulated heating demand equals the district heat demand⁶ while the cooling demand has to be provided by a chiller.⁷

The dry rooms are both supplied by an AHU each containing fans, cooling coils for pre-cooling of the outside air (supplied by the chiller), a desiccant wheel, a heating coil for heating of the dried air to the desired room temperature (district heating), a heating coil for the regeneration air flow (gas), and a waste heat recovery from the regeneration air. In order to estimate the power demand of the dry room operation, a model is derived based on power measurements⁸ and the analysis of the control scheme. First measurements have shown a rather constant gas demand⁹ during dry room operation as well as a constant power demand for ventilation. In addition, a regression analysis was conducted to investigate the correlation between the outside temperature and the power demand of the chiller. Figure 6.7 shows a scatter plot of samples for the power demand during intervals with an average temperature. It also shows a fit based on a polynomial function, which was implemented in the chiller model to estimate the power demand depending on the outside temperature.¹⁰

The effects of moisture emissions of workers and the relative humidity of the outside air on the energy demand of the dry room components were not considered. However, due to the structure of the dehumidification system, it is assumed that

⁶It was assumed that heat supply is available throughout the entire year although it might be turned off during summer months.

⁷The model determines the required cooling demand to maintain the zone temperature in the desired range. However, in the BLB, the capacity of the available chiller is not large enough to supply the dry room AHU as well as to provide cooling for all zones.

⁸Measurements were only available for April, August, September and October.

⁹Approximately 7 m³/h. However, due to the lack of sufficient data, this aspect is neglected in the model so far.

¹⁰Goodness of fit: R-square: 0.8496. The quality of this fit has to be re-evaluated if more data samples are available.

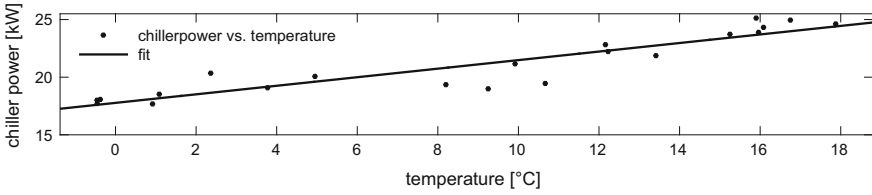
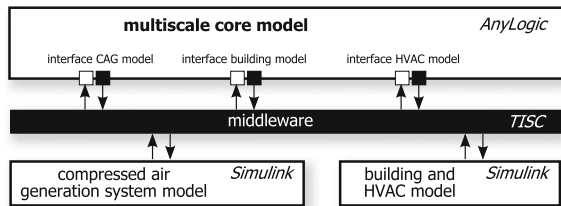


Fig. 6.7 Scatter plot of samples of chiller power demand [kW] and outside air temperature (°C)

Fig. 6.8 Model coupling structure



higher internal moisture loads and higher outside air humidity would result in a higher gas demand.¹¹ Moreover, in addition to the use of constant values (e.g. as for the ventilation power demand) or empirical model (e.g. as for the chiller power demand), it is also possible to calculate the theoretical energy demands based on the specific characteristics of the air streams to and from the dry room. Such detailed modeling may be reasonable for system or control design or to accurately determine the indoor conditions. However, it would require further in-depth knowledge about the dehumidification and ventilation system and cause higher modeling effort.

Model Coupling

The building model and the compressed air system model are connected to the core model via the middleware TISC, as shown in Fig. 6.8. The building model receives information from the process chain model about the shift schedule and variables about heat emissions for each building zone. In return, the building model provides the temperatures for each zone, the heating and cooling demands, as well as the power demand of the chiller. The zone temperatures are used in the core model to calculate the heat emissions of each machine. Furthermore, the building model provides the outside air temperature which is used to determine the power demand of the chiller of the air treatment system.

¹¹Further studies could deal with the measurement of the zone dew point temperature along with the number of people inside a dry room over a time period. This may enable to derive a regression function for the power demand depending on moisture loads.

6.1.4 *Verification and Validation (VI)*

The general verification of the core model, the compressed air system model, and the coupling via TISC was already explained in the previous chapter. The models used in this study were verified based on available production data and energy measurements. Since the BLB is usually not operating at full utilization, data about energy demands and control of HVAC systems are not completely available. Furthermore, the building and HVAC model was modeled without having complete data and information about system characteristics and control parameters. As an example for limitations, heat transfers between building zones are not considered and the materials of construction elements are not exactly matched with the materials used in the BLB. Moreover, the calculation of humidity is not included in the building model. However, the geometry of building zones is specified accurately and the model in general shows the expected thermal behavior. For example, the temperatures in larger zones change slower compared to zones with smaller air volume and zone temperatures increase if heat is emitted from internal heat sources (provided by the core model). Thus, the simulation results are useful as a rough estimation of the building climate and to highlight the directions of interdependencies between model parameters. In summary, although some models were verified and validated based on available data, the overall model cannot be considered validated and serves only as an experimental model demonstrating the functionality of the multiscale simulation.

6.1.5 *Definition (VII) and Execution (VIII) of Simulation Runs*

Specific simulation runs have to be defined based on the objectives and models have to be configured accordingly. In this study, different experiments are used to illustrate possible use-cases of the multiscale simulation. First, a reference scenario is defined which imitates one month of production of one type of battery cells. Jobs, product types, processing parameters, machine allocation and processing times were defined in order to create a consistent scenario of the cell production within the BLB.¹² Each job represents the production of 50 cells and it is assumed that one anode batch and one cathode batch are used for exactly these 50 cells. This reference scenario can be used as a benchmark to evaluate the effects of different system changes related to various planning tasks. This case study addresses the following five exemplary tasks:

T₁: Evaluation of different drying times and temperatures The coating and drying machine has a high power demand and relatively long processing times. It can be assumed that this machine is a bottleneck which effects the output of

¹²Since there is no established series production scenario of the BLB, this reference scenario represents one exemplary system configuration which is not necessarily completely representative for the BLB.

cells and causes high energy demands. It should be evaluated how the output and energy demand is effected by different processing times and temperature settings.

T₂: Evaluation of additional machines The reference scenario refers to the actual machine configuration of the BLB. However, since the BLB is not equipped for series production, it is expected that the material flow will be blocked and that buffers will run full due to limited capacity of some processes. For this reason, the simulation should enable evaluating if additional machines can improve the material flow and increase the output.

T₃: Evaluation of different solvents Electrode slurries can contain different solvents. Often NMP is used which is removed within the drying process and requires treatment of the exhaust air. If water is used as solvent, no air treatment is necessary. The effects of solvents on energy demands should be evaluated.

T₄: Evaluation of different weather conditions The reference scenario is simulated with weather data for July. It is of interest to evaluate how much the HVAC energy demands are effected by the outside air temperature.

These evaluation tasks are the basis for the derivation of simulation runs. Simulation runs represent scenarios with different production system and simulation model configurations. They have to be specified to generate simulation results which allow the evaluation of the related tasks. Table 6.1 lists the description of defined simulation runs for this case study. These runs have been executed to generate results.¹³

Table 6.1 Description of simulation runs

SR	Description
SR _{RS}	Simulation run for the reference scenario
SR _{1,1}	Reference scenario but with drying time increased by 10%
SR _{1,2}	Reference scenario but with drying time increased by 20%
SR _{1,3}	Reference scenario but with drying time reduced by 10%
SR _{1,4}	Reference scenario but with drying time reduced by 20%
SR _{1,5}	Reference scenario but with temperature at 100 °C
SR _{1,6}	Reference scenario but with temperature at 120 °C
SR _{2,1}	Reference scenario but with two filling machines
SR _{2,2}	Reference scenario but with two coating and drying machines
SR _{2,3}	Reference scenario but with two filling machines and two coating and drying machines
SR _{3,1}	Reference scenario with slurry containing NMP solvent. Air treatment system is activated
SR _{3,2}	Machine configuration from SR _{2,2} with slurry containing NMP solvent. Air treatment system is activated
SR _{4,1}	Reference scenario but with weather data for January
SR _{4,2}	SR _{2,3} but with weather data for January
SR _{4,3}	Reference scenario but with weather data for October
SR _{4,4}	SR _{2,3} but with weather data for October

¹³Each run starts with empty buffers and consequently not in steady state. In addition, stochastic effects such as machine failures or process variations are neglected due to the lack of required data.

6.1.6 Evaluation of Simulation Results (IX) and Objectives (X)

The results of the simulation runs were examined regarding result quality and usability for the evaluation of the defined tasks. Figure 6.9 presents exemplary plots of performance indicators of SR_{2,3} for the simulation period of one month. These plots show (from top to bottom) the power demands of machines, compressed air generation, heating and cooling, the dry room (ventilation and chiller), and lighting. These plots enable identifying trends and characteristic situations. For example, a daily power demand pattern can be identified from the first plot. Furthermore, heating demands are higher at times with lower outside temperature and cooling is only active during days with a higher outside temperature. In addition to these monthly plots, it is possible to visualize the total energy demand of each machine and system for the simulated month – as shown in Fig. 6.10 for SR_{2,3}. This visualization helps to identify the most relevant machines/systems. Here it becomes clear that the highest energy demands are caused by building cooling demand, coating and drying machines, the chiller for the dry rooms, as well as the ventilation of zones.

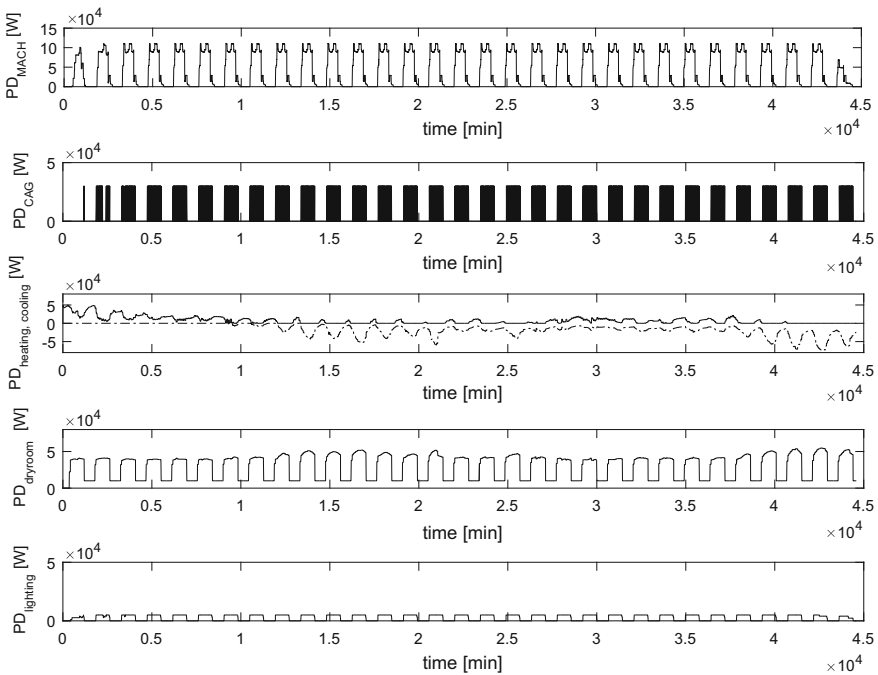


Fig. 6.9 Plots of indicators for SR_{2,3}. From *top to bottom*: power demand of machines, compressed air generation, heating and cooling, dry room, and lighting

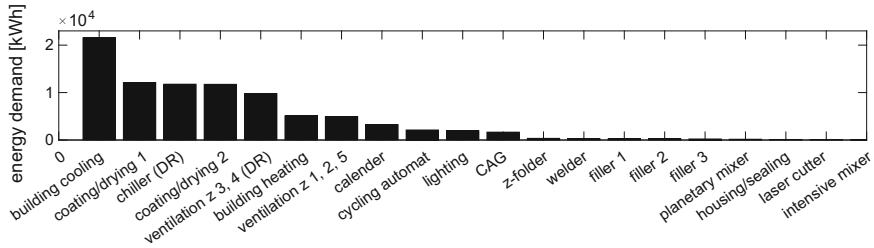


Fig. 6.10 Energy demands of machines and systems during one month for SR_{2,3}

In this case study, indicators have been selected for the comparison of simulation runs. These indicators were the yield of cells during the simulated period of one month, the utilization of the process chain (uti_{PC}), the mean production time per job (PT_{mean}) and its deviation (PT_{dev}), energy demands (ED) of different systems, as well as the average direct and indirect embodied energy per cell ($\emptyset DEE_{cell}$, $\emptyset IEE_{cell}$). Table 6.2 lists the results for the simulation runs. Even though the actual numerical values of the results must be doubted due to the non-validated model character, they enable a discussion of the individual measures, the comparison of simulation runs, and the improvement of the understanding of the complex behavior of the production system.

The results of the reference scenario SR_{RS} show that the mean of the production time per job is high with 189 h. A detailed analysis showed that the production time increased over the observed time period. This is caused by including the model warm up phase into the simulation results. After reaching a steady state, the model shows that the machines in cell assembly have full buffers because the filling process is a bottleneck. Many semi-finished product units are stored in buffers and cannot be finished due to limited machine capacities. Furthermore, the mixing processes are often blocked which allows to conclude that the coating and drying machine is also a bottleneck. However, the sole extension of coating and drying capacities would only result in more buffered semi-finished product units in cell assembly. In summary, the high mean production time indicates a large amount of work in progress and an undesired obstructed material flow.

The results of SR_{1,1}–SR_{1,4} show the effects of different processing times for coating and drying. As expected, longer processing times result in higher energy demands of machines and higher direct embodied energy per cell. The reduced mean production time of SR_{1,2} compared to SR_{1,1} can be explained with fewer started jobs due to not available coating capacities. Thus, fewer product units fill the buffers in cell assembly causing shorter production times. The opposite effect shows in SR_{1,4}: A shorter time for coating and drying increases the yield because the cell assembly can start earlier within the simulated month. On the downside, higher throughput in electrode production fills the buffers in cell assembly more quickly causing the production times to increase even more for later jobs and blocking of the previous processes. The resulting reduced activity in electrode production results in lower

Table 6.2 Results of simulation runs

SR	Yield	PT _{mean} (h)	PT _{dev} (h)	ED _{TOTAL} (kWh)	ED _{MACH} (kWh)	ED _{CAG} (kWh)	ED _{HVAC} (kWh)	ED _{LIGHTS} (kWh)	∅ DEE _{cell} (kWh)	∅ IEE _{cell} (kWh)
SR _{RS}	1129	189	58.9	57,003	17,030	878	36,760	1,905	11,292	39,198
SR _{1,1}	1129	189	58.8	58,272	18,303	873	37,218	1,877	11,995	39,619
SR _{1,2}	1107	186	53	59,146	18,949	863	37,478	1,854	12,973	40,455
SR _{1,3}	1129	189	59	55,166	15,907	887	36,501	1,870	10,583	38,28
SR _{1,4}	1136	249	109	54,333	14,627	1,014	37,079	1,612	10,466	37,362
SR _{1,5}	1129	189	59	72,675	28,639	878	41,253	1,905	17,008	47,634
SR _{1,6}	1129	189	59	81,654	34,570	878	44,300	1,905	20,223	52,101
SR _{2,1}	1485	96	14	55,268	16,156	868	36,645	1,589	10,342	26,875
SR _{2,2}	1140	292	137	57,919	17,095	1,039	38,348	1,435	11,878	38,928
SR _{2,3}	2845	87	13.5	78,106	30,885	1,665	43,660	1,934	9.91	17,543
SR _{3,1}	1129	189	59	66,593	26,880	1,049	36,759	1,905	16,675	42,309
SR _{3,2}	1485	96	14	65,324	26,013	1,037	36,661	1,611	15.93	28.06
SR _{4,1}	1129	189	59	101,392	17,029	878	81,579	1,905	11,292	78,516
SR _{4,2}	2845	87	13.5	103,756	30,885	1,655	69,310	1,934	9.91	26.56
SR _{4,3}	1129	189	59	73,433	17,029	878	53,620	1,905	11,292	53,751
SR _{4,4}	2845	87	13.5	64,746	30,885	1,655	46,547	1,934	9.91	17,947

overall energy demands while maintaining a similar yield compared to the previous simulation runs. However, the amount of produced electrodes is lower at the end of one month.

SR_{1,5}–SR_{1,6} differ from the reference scenario only regarding the power demand for the coating and drying machine. The results show the expected higher energy demand of machines but also of HVAC systems due to higher cooling demands. Consequently, the direct and indirect embodied energy per cell is effected noticeably by the drying temperature.

SR_{2,1}–SR_{2,3} examined the impacts of additional machines. First, in SR_{2,1}, two additional filling machines resulted in a higher yield due to a resolved bottleneck at the end of the process chain. The mean production time dropped significantly. The utilization of cell assembly was reduced (since buffers were not always filled and machines were in idle mode) which can be seen at the reduced power demand for compressed air generation. As a result of the higher yield, the indirect embodied energy per cell was noticeably reduced because the fixed power demands could be allocated to more cells. In SR_{2,2}, the reference scenario was extended by a second coating and drying machine. The results indicate that the bottleneck was not eliminated since the mean production time is very high and the yield similar to the reference case. In SR_{2,3}, the reference scenario was extended by both two additional filling machines and one additional coating and drying machine. The results show that a higher yield and shorter production times were possible in this case. This underlines that the cell assembly was not fully utilized in SR_{2,1}.

The results of SR_{3,1} show – in comparison to the reference scenario – that the air treatment system caused higher overall energy demand as well as higher direct (increased by almost 50%) and indirect embodied energy per cell. SR_{3,2} revealed – based on SR_{2,1} – that a higher output did not help to reduce the embodied energy since the energy demands of the air treatment system were assigned to the coating machine. If the energy demand of the air treatment system would have been allocated to the TBS systems, the higher output in SR_{3,1} would have resulted in reduced indirect embodied energy compared to SR_{3,1}. It can be concluded that avoiding NMP solvents is an important measure in reducing the overall energy demand.

SR_{4,1} and SR_{4,2} used weather data for January. The high required heating demands caused an increase of the total energy demand and indirect embodied energy per cell. Even though the output of SR_{4,2} is higher, the indirect embodied energy is still significantly higher compared to SR_{2,3}. SR_{4,3} and SR_{4,4} used weather data for October. The weather conditions caused lower heating and cooling demands due to moderate temperatures.

The embodied energy per battery cell is an important indicator for the evaluation of the environmental impacts of each cell. Figure 6.11 presents the simulation results for the average direct (DEE) and indirect (IEE) embodied energy of one battery cell. It becomes clear that the indirect embodied energy was higher in all simulation runs. Furthermore, the indirect embodied energy strongly depends on the yield of finished cells. This means that the energy demands of peripheral equipment and TBS as well as the yield of a factory must be considered in the economic and environmental assessment of battery cells. Moreover, the simulation results allow a breakdown

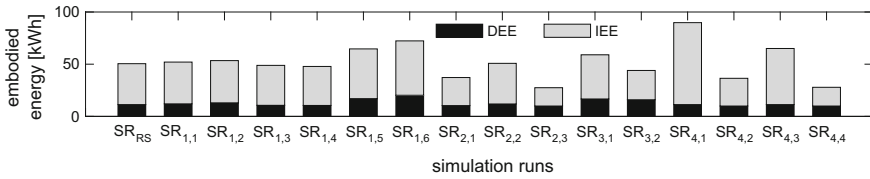


Fig. 6.11 Average direct (DEE) and indirect (IEE) embodied energy per battery cell

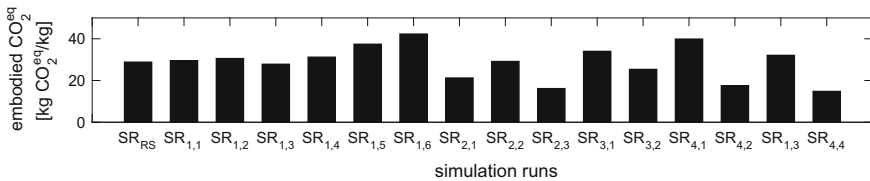


Fig. 6.12 Average embodied equivalent CO₂ emissions from energy supply per battery cell

of the energy demand into different energy carriers. This enables a more accurate determination of environmental impacts and energy costs. For example, in this study the building heating is supplied by district heat while the other machines and TBS systems demand electricity. These energy carriers cause different specific equivalent CO₂ emissions¹⁴ which can be used to determine the average embodied equivalent CO₂ emissions from energy supply for each produced battery cell, as shown in Fig. 6.12.

In summary, the results allow to draw some general conclusions. The processing times of individual processes may effect the bottleneck(s) of a process chain and influence the achievable yield of finished cells. This further influences the indirect embodied energy per cell. Moreover, the energy demands of processes may depend on product specifications (e.g. type of solvent) and process parameters (e.g. temperature settings). As an example, the usage of NMP solvent increases the energy demand noticeably (SR_{3,1} and SR_{3,2}). This also effects the direct embodied energy per cell. In addition, weather conditions have a significant effect on the energy demand of HVAC systems. Thus, weather conditions have to be considered while selecting a location for a battery cell factory.

Overall, the developed models can be used to conduct simulation runs for further planning tasks or for in-depth sensitivity analysis of single parameters or model characteristics. Moreover, the model functions allow the analysis of worker behavior, value streams of jobs, the development of product characteristics, etc. These aspects were not included in this case study but could be used for future studies.

¹⁴For Germany: CO₂^{eq} impact of electricity production: 609 g/kWh (Umweltbundesamt 2015); CO₂^{eq} of district heat (from fossil energy carriers): 325 g/kWh (Umweltbundesamt 2013).

6.2 Simulation of Module Assembly

In this second case study, a simulation model was created for the assembly of battery modules. This demonstration focused the application of the multiscale core model for the evaluation of different process chain configurations. For simplification, only the process chain scale with workstations¹⁵ was examined neglecting processes, workers, TBS, and the building. Due to this specific focus, this section does not specifically cover each step of the application procedure.

Problem Formulation and Objective Definition

The scope of this study was the comparison of a traditional assembly line configuration with a matrix-structured process chain layout for the simultaneous assembly of three exemplary types of battery modules. These modules differ regarding the number of cells, installed cables and sensors, geometric dimensions, and the housing. Consequently, although the production steps of all considered module types are in general identical, there are differences in the exact production steps and related processing times. In this case, two module types require eight production steps while the third requires seven steps because it does not contain a cooling system. Table 6.3 lists the production steps with related processing times for the three module types.¹⁶

The differing processing times of production steps result in starving and blocking of workstations. Thus, the goal of the production planning is defining process chain layouts and machine allocations which enable a high system utilization by avoiding starving and blocking. The objective of the simulation study was testing of different process chain layouts, different buffer sizes of workstations, and different allocations of production steps to workstations.

Table 6.3 Production steps with related processing times for each module type

	Processing time per production step (min)							
	PS ₁	PS ₂	PS ₃	PS ₄	PS ₅	PS ₆	PS ₇	PS ₈
Module type 1	3	5	7	5	4	5	6	5
Module type 2	4	6	8.5	6.3	4	6	6	5
Module type 3	2.5	4.5	5	3	5	–	5	5

¹⁵In this case study, the term workstation was used since assembly tasks are often manual tasks which are supported by different tools or resources.

¹⁶The processing times are defined based on assumptions and serve the purpose of demonstration. They do not reflect real-world production data.

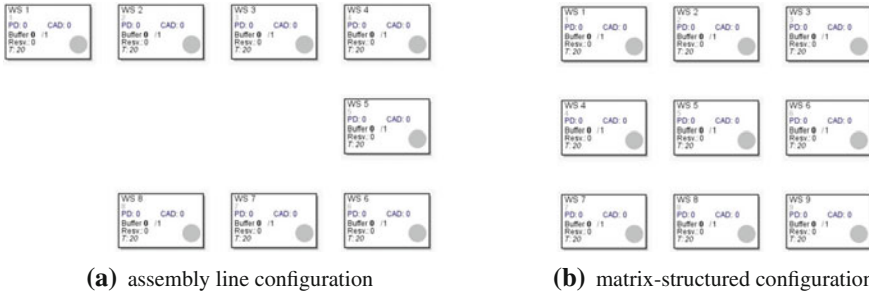


Fig. 6.13 Screenshots of the assembly line configuration in u-shape (a) and the matrix-structured configuration (b) modeled in AnyLogic

Development of Models and Implementation

The multiscale core model was used for modeling of different process chain configurations and for evaluating scenarios regarding utilization and production time. In the model, the assembly line configuration and the matrix-structured configurations were created by specifying the workstation coordinates as well as the allocation of production steps to workstation. The operational states of workstations were represented by generic machine models. Energy demands were not observed in this study. Moreover, shift hours were not considered since TBS systems are not modeled and there are no effects of weather conditions on any production system element. Battery modules were represented by processing unit agents and the control strategy shortest throughput time was used to control the flow of processing units.

For the assembly line configuration, each production step was allocated to one workstation. Hence, in this case there were eight workstations which were positioned within the virtual shop floor coordinate system according to the order of production steps. Each workstation must have the required resources (e.g. tools).

For the matrix-structured configuration, each production step was allocated to multiple workstations based on different criteria. For example, if different production steps require the same tools (e.g. for fixation of cells on a base plate and for mounting of the housing), these production steps can be allocated to the same workstation. In this study, the production steps were allocated to nine workstations. Figure 6.13a, b present screenshots of the implemented process chains configurations.

Definition and Execution of Simulation Runs

The simulation model was used to determine the utilization and total production time for the assembly line and the matrix-structured configuration. For each configuration, the assembly of 500 modules was simulated in one simulation run with a random sequence of product types. The buffer size of each workstation was set to one. A fixed seed value was used for simulation in order to replicate the same sequence of products for each simulation run. This random sequence of product types should represent unknown demands for each product type. After the first two simulation

runs for both the line and matrix-structured configuration, a third run was executed to analyze an optimized matrix-structured configuration.

Evaluation of Simulation Results and Objectives

The results of the simulation runs were analyzed regarding the indicators utilization and overall production time for the simulated assembly of 500 modules. Figure 6.14 shows the plot of the utilization for the assembly line and matrix-structured configuration. The plots for both configurations show a fluctuation of the utilization which can be explained by regular starving and blocking of workstations. However, the utilization of the matrix-structured configuration (mean: 78.8%) is higher compared to the utilization of the assembly line configuration (mean: 69.5%). Moreover, the required production time for 500 modules is approximately 20% shorter with the matrix-structured configuration (including ramp-up and ramp-down of the assembly activity).

For further optimization of the matrix-structured configuration, the causes of blocking were investigated. A total of 186 blockings occurred during the simulation run. It was analyzed in which state a processing units could not be forwarded to a next workstation. A histogram was created showing the production step of processing units at which blocking occurred. This indicated which production steps were not sufficiently available in the process chain. Figure 6.15 presents the histogram which shows that processing units are often blocked after production step PS₄ and PS₇. Consequently, workstations for production step PS₅ and PS₈ were not available when needed. As a solution, these both production steps were additionally allocated to workstation 9. Another simulation run was executed to evaluate this change in production step allocations. Figure 6.16 presents the plot of the resulting utilization of the adjusted matrix-structured configuration in comparison to the previous simulation results of the initial matrix-structured configuration. The adjusted matrix-structured configuration resulted in a slightly higher utilization (mean: 81.6%) and a shorter production time. The total number of blockings was reduced to 49. This procedure

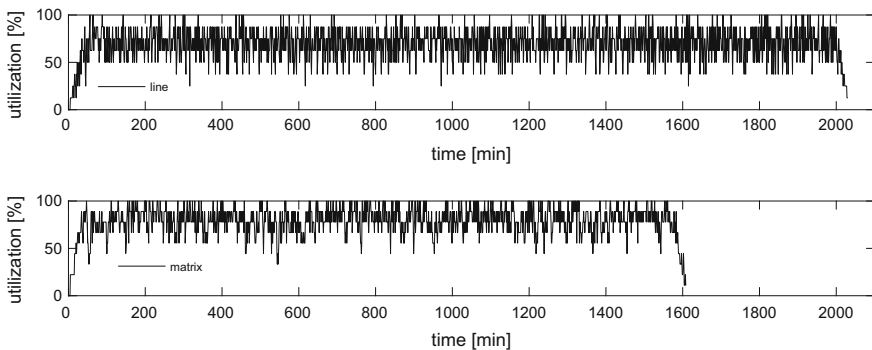


Fig. 6.14 Simulation results: Utilization of assembly line (*top*) and matrix-structured configuration (*bottom*)

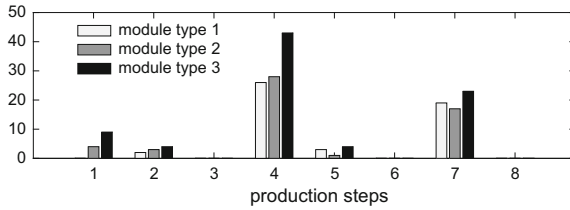


Fig. 6.15 Histogram of blockings per production step

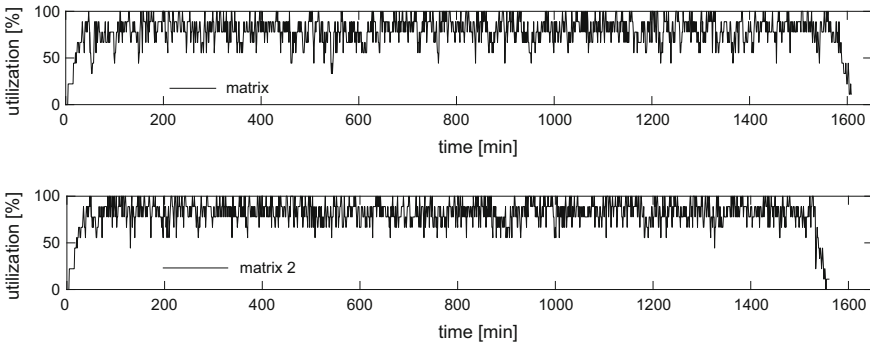


Fig. 6.16 Simulation results: Utilization of the initial (*top*) and the adjusted matrix-structured configuration (*bottom*)

for analyzing blockings could be repeated in order to further optimize the allocation of production steps. Alternatively to the additional allocation of production steps to other workstations, buffer sizes may be increased or new workstations added to the assembly system. The effects of such improvement measures can be analyzed with the simulation model.

The core model could also be configured for the consideration of machine failures. Probability distribution could be used to model the times between the occurrence of machine failures (MTTF) and until failures are repaired (MTTR). The model must be used to execute a large number of simulation runs with random seed value in order to address the implemented stochastic effects and to avoid a snap-shot character of simulation results. It was shown in Schönemann et al. (2015) that matrix-structured assembly systems can be more suitable for handling stochastic machine failures in comparison to sequential assembly lines. In the analyzed scenario, an assembly line configuration was compared to a matrix-structured configuration. The failure behavior of each machine was specified by Weibull functions for MTTF and uniform distributions for MTTR. Weibull functions have been used since they are adjustable to individual machine behavior. The uniform distribution allowed to equally consider short and long repair times. The model was used to execute 100 simulation runs with random seed values of the random number generator. The results show a higher

utilization of the matrix-structured configuration which was equally high compared to the deterministic case without machine failures.

In summary, this second case study has shown how the process chain model can be used to evaluate different process chain configurations. The shown evaluation addressed the economic performance of an assembly system by analyzing the system utilization and the production time for a predefined yield. Such analysis of the process chain performance may also be applied to cell production in the case that multiple redundant machines are available. Moreover, in further simulation runs, a modeled process chain of an assembly system can also be embedded within a factory environment and extended by detailed models for processes, TBS, and the building – similar to the demonstration in the first case study.

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Chapter 7

Summary and Outlook

This chapter summarizes the presented work (Sect. 7.1), gives a critical review of the achieved results (Sect. 7.2), and provides an outlook by suggesting further research (Sect. 7.3).

7.1 Summary

The presented work aimed at contributing to the research field of production system simulation in general and simulation of battery production in particular. Chapter 1 presented an introduction to the challenges in battery production and highlighted the motivation for a multiscale simulation approach for production systems.

Chapter 2 discussed the required background information about battery production and simulation. In its first part, the chapter separately covered the structure and components of battery systems as well as the principles of production systems before presenting the specific characteristics and requirements of the production of battery electrodes, cells, modules, and systems. In the second part, the chapter discussed the simulation methodology in the context of the digital factory network and introduced different modeling characteristics, simulation approaches, and procedures for simulation studies. The idea of a multiscale simulation for production system was derived and various approaches for parallel or co-simulation were presented which enable the simulation of multiple scales. The chapter ended with a summary about the requirements for the simulation of battery production systems. In short: The production of electrodes and cells is characterized by specialized unit processes which have strong influences on cell performance, requires expensive and energy intensive machines, and demands for defined environmental conditions. The assembly of modules and systems is characterized by assembly tasks, a high product variety, and the demand for a flexible material flow. Consequently, a multiscale simulation approach must

consider unit processes, material flow in process chains, TBS, and the building, as well as the impacts of processes on product characteristics.

Chapter 3 analyzed existing contributions in research fields related or relevant to multiscale simulation in production. It showed that there are various simulation concepts combining the simulation of different production system scales, addressing different objectives (technical, economic, environmental), and using different simulation approaches. However, the found simulation concepts mostly focus on specific planning problems and do not enable the multiscale simulation of a whole production system. None of the identified and evaluated contributions allowed or suggested a detailed simulation simultaneously considering the influences of processes on product characteristics, energy and material demands of unit processes, the material flow in process chains based on a defined schedule, interactions between machines and TBS, and the effects of outside weather conditions and the building shell construction on inside ambient conditions. Since such multiscale approach would support the improvement of battery production, Chap. 3 ended with the formulation of a research demand.

Chapter 4 described the proposed multiscale simulation concept for battery production in greater detail. It began with the definition of objectives and requirements based on the identified research demand and the initial motivation to develop a new modeling approach. The chapter continued describing the derivation of system boundaries and a generic modeling framework for a multiscale simulation as a pattern for structuring interfaces between required models. Based on this framework, the required models were derived and explained in detail. The process chain model was found to be the central element of a multiscale simulation approach for production systems since it determines the activity within a production system and acts as a coordinator for other models. Concepts were presented for a process chain model with the desired functionality as well as for additional detailed models for machines, products and processes, TBS systems, and the building. For each model type, the description describes the inputs from and outputs to other models. These intersections between models were summarized and it was shown how detailed models can be integrated or coupled to the process chain model in order to exchange the specified information. Since the coordinated use of simulation models delivers a great amount of results, the multiscale simulation concept further suggests indicators and representations for the evaluation and visualization of simulation results. Finally, an application procedure with twelve generic steps was proposed which supports the development, maintenance, and employment of multiscale simulations for specific production systems. It was suggested to define a responsible organizational role for the coordination of involved stakeholders and the monitoring of the application procedure.

Chapter 5 covered the implementation of a multiscale core model with interfaces for external models based on the derived functionality described in Chap. 4. The chapter presented the model architecture and details of the model components. In addition, as an example of an external model, a generic compressed air generation system was implemented and connected to the multiscale core model via a middleware software. The final section of the chapter explained the verification of the internal functions of the process chain model as well as relevant aspects regarding

the coupling of external models such as simulation step size and synchronization time. As demonstrated by examples, these both aspects may influence the accuracy of simulation results.

Chapter 6 presented an exemplary application of the multiscale simulation concept and the developed model infrastructure around the multiscale core model. Two case studies provided insight into the application procedure, model functions, possible use-cases and exemplary simulation results. The first study addressed the battery cell production and put emphasis on the multiscale character including detailed models for products, machines, TBS, and a building. It was shown how the multiscale model can be used for specific evaluation tasks. The simulation results revealed relations between different system elements and improvement measures highlighting the necessity to consider the complex system dynamics for the evaluation of isolated measures. Some key findings indicate that increasing the output is important to reduce the production cost and environmental impacts due to high fixed energy demands which are independent from the production rate. Furthermore, weather conditions have noticeable effects on these fixed energy demands. Thus, selecting a factory location has to consider the demand for moderate outside temperatures in order to avoid high heating or cooling demands. The second study addressed the assembly of battery modules focusing on the analysis of different process chain configurations. In particular, a conventional assembly line was compared to a matrix-structured assembly system configuration for the assembly of different product types. The results show that the matrix-structured system can achieve a higher utilization while handling high product variety. Both case studies presented different selected application scenarios for the proposed simulation approach.

7.2 Critical Review

The presented simulation concept supports the development of multiscale simulation applications for production systems. The concept was derived from the defined objectives and extends the state of research by providing a generic modeling framework for multiscale simulations, the definition of required models for production system elements and their connecting interfaces, specific detailed modeling solutions, as well as an application procedure. Although the basic idea of comprehensive holistic production system simulations is not new, the proposed concept is unique in its proposition to combine economic, environmental, and technological objectives considering various scales from single product units to the building shell. This simulation concept was created in particular for the case of battery production but also provides helpful advice and hints for the development of multiscale simulations for any kind of production system. Especially the framework and the defined variables for information exchange between models are helpful for developers of multiscale production simulations for determining the required model functionality. Moreover, these presented concepts for detailed models for system elements may serve as a foundation for the development of specific simulation models. These aspects dif-

ferentiate the proposed concept from most of the identified research contributions which mainly presented exemplary applications and focused on selected objectives, production system elements or scales, and simulation methods. However, it has to be recognized that the concepts for detailed models are of simplified nature and – in particular for HVAC systems, buildings, and processes – only qualitatively described. This is due the fact that it is difficult to create generic models which are valid for any kind of specific system.

An important feature of the multiscale simulation concept is the suggested use of a process chain oriented core model as a coordinator for other models. This allows imitating a realistic production activity and to dispense the use of average values or assumptions for operational times and demands of system elements (e.g. machines). Furthermore, a process chain simulation enables evaluating economic objectives such as system utilization and production times as well as allocating of all determined energy demands to the achieved yield. Such use of a process chain model in coupled simulations was already suggested for example by Hesselbach et al. (2008) and Junge (2007). However, the benefit of the here proposed multiscale core model is the flexible agent based modeling approach. The approach considers product units (or batches) and machines as agents with individual properties, objectives, and requirements. This enables the flexible configuration of different process chains, product types, control strategies for product routing, machine allocation, and the tracking of product characteristics (e.g. material input, quality parameters, embodied energy) along a process chain. The flexibility in modeling is important for the simulation of battery production since it facilitates the adaptation of a developed multiscale simulation to new production technologies and process chain configurations which are expected to come along with the establishment of new battery technologies. Moreover, in contrast to traditional process chain simulations – which are based on DE models considering products as events and not as instances with individual properties – the agent based approach allows to set individual product characteristics after each process and to carry this information as inputs for following processes. This makes it possible to study the amplifying or damping effects of variations in processing results along a process chain. Thus, the proposed process chain model represents an innovative approach which may also be interesting and useful for process chain simulations addressing solely issues of product quality or production cost.

An exemplary multiscale core model was implemented with interfaces to external models. This model is a generic tool which can be used to create simulation applications for specific cases by connecting external models of machines, products and processes, TBS, and buildings. It demonstrates how a process chain model functionality is suitable for the coordination function in a multi-model environment of coupled co-simulation applications. This tool could be used for the simulation of battery production systems but is also adaptable to any other kind of discrete production activity. However, although the model was build with care and considering the required functionality defined in the concept, it has to be kept in mind that the tool is a functional prototype and no finished software product.

The concept and the implemented core model were exemplary applied in two academic case studies. These applications showed that a multiscale simulation can

support various planning tasks in battery production and that it is applicable for different production stages such as cell production and module assembly. It becomes clear that a multiscale simulation is able to generate results which would not be possible in this extent by isolated simulation models. Within the case studies, detailed specific models have been created for machines, HVAC systems, and a building shell. These models only serve the purpose of demonstration but cannot be expected to deliver valid results due to the lack of data and in-depth knowledge about the simulated systems. For the same reason, the case studies neglected some relevant functions of the concept. Examples are the consideration of material demands, machine-hour rates, process models including machine tolerances, stochastic effects such as machine breakdowns, or influences of moisture loads on the energy demand of the dry rooms. In addition, the case studies do not related to mass production systems. The first study covered the cell production within a research facility and the second study addressed an abstract module assembly process chain. Although the application of the simulation concept could be elaborated and the results are assumed to be transferable to larger productions systems, this situation has to be kept in mind. For a real case application, it is necessary to acquire a sufficient amount of data about the production system and to develop valid models utilizing expert simulation knowledge and involving all stakeholders. The proposed application procedure supports these tasks.

Overall, the multiscale simulation concept brings various advantages for the simulation of battery production systems. The flexible agent based process chain simulation combined with the modular architecture achieved by the coupling of different models creates a planning tool which can be adapted to different scenarios and new technologies. Consequently, this one method can be used for various planning tasks and adapted to future production system configurations. Moreover, it provides a modeling concept which fosters an in-depth understanding of the observed production system. Nevertheless, although the concept fulfills the set objectives and requirements, it is necessary to mention a last relevant challenge. Multiscale simulations bear the risk of being very complex and causing huge efforts for model development and employment. Beside the resulting resource demands, this high complexity may give the impression that the results are more accurate and useful than they actually are. The case studies have shown that many assumptions and simplifications are necessary to create a manageable model which can be executed in acceptable time. These simplifications and assumptions may effect the results and could lead to wrong conclusions and a reduced acceptance of the results. However, this challenge should not impair the potential and relevance of multiscale simulation applications for production systems. In contrast, further research should be motivated to find solutions for new efficient modeling and simulation techniques, as well as methods for knowledge discovery to create valid models for processes and systems more easily.

7.3 Outlook on Further Research

Further research activities can build upon the presented work and contribute to the successful establishment of multiscale simulations for production systems in general and for its application to battery production in particular.

Model library for machines and equipment The composition of a multiscale simulation and the achievable results depend strongly on the available models of system elements. The simulation concept and the proposed framework for model coupling state which models are required to consider all relevant production system elements. In the context of the work, different models for machines and equipment (e.g. TBS systems) were developed and implemented for the use in a multiscale simulation. However, these models are of generic character or based on real machines for the small scale cell production in the BLB. Moreover, detailed models are not available for all relevant system elements. Consequently, it is of interest to create a library of valid models for machines and equipment used in series production which can be employed to create multiscale simulations of various large scale production systems. This task requires information about the used production equipment with related characteristics (e.g. capacities, processing times, machine-hour rates, etc.) in industry along and intensive energy data measurements. Such library, supplied with knowledge from different disciplines, could be an important measure in the context of the digital factory.

Product characteristics and process models The multiscale core model provides the functionality to apply process models within machine model agents and to determine product characteristics which can be stored in processing unit agents. This would allow evaluating the effect of processes (e.g. variations due to tolerances) on product characteristics and to create transparency about the effects along a whole process chain. However, the discussion of product characteristics and process variations in this work stayed on a rather theoretical level due to the lack of real data about machine and process tolerances. Since this aspect is of great interest for achieving a high product quality at low cost, the described ideas should motivate further work in this direction. In particular, it is important to develop models for each process which define how a process creates or modifies product characteristics. This requires empirical studies about production processes and the derivation of knowledge from the gathered data. It is necessary to identify the influences of process parameters, machine properties, and environmental conditions on the process stability and resulting product characteristics. The development of process models is a task for process experts but it should be accompanied by developers of a multiscale production simulation to guarantee the usability of the resulting models.

Coupling of process simulation Process models can be of various types. Some processes might be replicated virtually by simulation models which simulate the transformation of process inputs for given process parameters over the processing time. Such model – for example based on DEM – may enable to consider various influences on the process execution and resulting product characteristics. Thus,

integrating such models into a multiscale simulation may improve the consideration of product quality. However, process simulation models may require long time for execution. It should be tested if the execution times of available process simulation models allow a co-simulation with the process chain model.

Combination with battery simulation If a multiscale simulation of a production system for battery components is able to simulate process variations and resulting product characteristics along a process chain, it is possible to use the resulting product characteristics of finished product units as input values for battery simulation models. This enables the evaluation of the influences of process tolerances on battery performance. In particular for battery cells such approach is promising since experimental parameter variations within each process of a process chain cause high efforts. A multiscale simulation of production allows to use data and models for each isolated process and to virtually imitate the effect of tolerances along an entire process chain. A connected battery model could simulate the performance of produced cells and determine critical influencing characteristics resulting from production of which other tolerances may be again examined by the process chain simulation. This supports the simultaneous improvement of battery design and production operation.

Adaptation for reverse material flows The multiscale simulation approach can be adapted for the evaluation of recycling systems. The developed simulation concept allows also to model diverging reverse material flows and recycling processes in detail. A similar application was already presented by Colledani and Tolio (2013).

Superordinate system dynamics model The simulation of battery production systems could be extended by a subordinate system dynamics model for the assessment of a network of production facilities. Such model could describe the demand, supply, supply chain operation and market response to new technologies. It could be fed with results from the multiscale production system simulation (e.g. possible output per time period) and in return provide results as input for the simulated production program (e.g. the demands for different product types).

Application to other industrial sectors Although the concept was developed for the production of batteries, it has been kept in mind that it is also applicable for other production systems and industries. It will be an interesting task to use the concept and developed modeling logic for different case studies in order to evaluate the transferability. Furthermore, it would be interesting to adapt this approach to the process industry with continuous product flows. A test case could be the production of carbon fibers which require different processing steps with very high temperatures and energy demands. Solutions must be found for the assignment of product characteristics to fractions of continuously produced products (similar to the coating and drying of electrodes).

Data mining Valid data from real applications are important inputs for simulation models. Big data applications and data mining approaches are becoming more established in research and industry. It is recommended to combine data acquisition and analytic applications with simulation models. The developed multiscale simulation allows to use data for specific simulation models. In addition to the

application of data mining methods for the generation of simulation inputs, these methods can also be used for the evaluation of simulation results. Especially if a multiscale model is very detailed and considers many elements of a production system, data mining can be helpful to identify patterns within the generated results.

Commercial software solutions The functional prototype of the multiscale core model with interfaces for external models must be further developed for a broad application in industry and research. It is important to achieve a better user interaction and a workflow based on industry standards for software tools. Alternatively, established software for process chain simulation (such as Plant Simulation or Arena) could be extended with interfaces for external models or middleware software. In general, it is important to establish the technical feasibility to connect simulation models which are implemented in different software tools. This would foster the re-usability of created simulation models, which is a major barrier for the broad application of simulation in industry.

Simulation-based production control Simulation models could be used for operational production planning by providing predictive and real-time simulation results in order to control the actual production system operation. The multiscale simulation approach enables the development of a complete factory model which could be used for simulation-based production system control if the required computational resources and interfaces to control tools are available.

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