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Hybrid modeling and forecasting of the energy and media demand in the beverage industry

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Content

Scientific Contributions

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The results and publications of this thesis were developed at the Technical University of Munich, Chair of Food Packaging Technology / Chair of Brewing and Beverage Technology from October 2016 to December 2021.

Full Papers

The following peer-reviewed publications were generated in the period of this work and are related to the topic of the thesis.
The doctoral candidate is the main author of the four publications presented in this thesis and shares in the fundamental and major part of the conceptualization, methodology, software development, validation, formal analysis, investigation, data curation and visualizations. The writing of the original drafts of the manuscripts is exclusively his product.

1. **Bär, Raik**; Voigt, Tobias. **Analysis and Prediction Methods for Energy Efficiency and Media Demand in the Beverage Industry**. Food Eng. Rev. 2019, 11, 200–217; DOI: 10.1007/s12393-019-09195-y. Impact Factor (5-year): 6.813.

2. **Bär, Raik**; Voigt, Tobias. **A metamodeling approach for the simulation of energy and media demand for the brewing industry**. Journal of Advanced Manufacturing and Processing. 2021, 3; DOI: 10.1002/amp2.10080.

3. **Bär, Raik**; Zeilmann, Michael; Nophut, Christoph; Kleinert, Joachim; Beyer, Karsten; Voigt, Tobias. **Simulation of Energy and Media Demand of Beverage Bottling Plants by Automatic Model Generation**. Sustainability 2021, 13, 10089; DOI: 10.3390/su131810089. Impact Factor: 3.251.

4. **Bär, Raik**; Schmid, Sebastian; Zeilmann, Michael; Kleinert, Joachim; Beyer, Karsten; Glas, Karl; Voigt, Tobias. **Simulation of Energy and Media Demand of Batch-Oriented Production Systems in the Beverage Industry**. Sustainability 2022, 14(3), 1599, DOI: 10.3390/su14031599. Impact Factor: 3.251.

Conferences and presentations with the first authorship

1. Modellierung und Simulation von Energie und Medienverbräuchen in der Brauerei. FREISINGER TAGE: Digitalisierung in der Lebensmittelwertschöpfungskette Webkonferenz, 30.06.2020

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Abbreviations

ANSI	American National Standards Institute
BPMN	Business Process Modeling Notation
CIP	Cleaning in Place
EES	Engineering Equation Solver
hl	Hectoliter
IoT	Internet of Things
ISA	International Society of Automation
MDSD	Model-Driven Software Development
MES	Manufacturing Execution System
MES-ML	MES Modeling Language
OMG	Object Management Group
PCS	Process Control System
SME	Small and medium-sized enterprises
UML	Unified Modeling Language
UN	United Nations
VDI	Verein Deutscher Ingenieure
WS	Weihenstephan Standards
XML	Extensible Markup Language
XSD	XML Schema Definition

Summary

The beverage industry is particularly challenged to produce sustainably and efficiently due to rising prices for energy and electricity, as well as economic, environmental, social and political conditions, such as the adoption of the United Nations (UN) Sustainable Development Goals. The energy-intensive production within the brewery, which is characterized by complex and hybrid process chains as well as a variety of different machines, represents a good example for the beverage industry. Especially for small and medium-sized enterprises (SMEs), there are specific barriers such as lack of time, capital and know-how to identify potentials to increase energy efficiency and to take appropriate measures. IT-based approaches can overcome these barriers and offer decision-makers the opportunity to pursue numerous approaches and make informed decisions. However, there is currently no solution that allows for a holistic analysis and forecast of the energy and media demand of hybrid production in the beverage industry and is also suitable for use in SMEs. Up to now, approaches have only focused on partial areas and individual aspects and are characterized by a high degree of complexity.

In this thesis, a method for the holistic and hybrid mapping, simulation and forecasting of the energy and media demand in the beverage industry, using the brewery as an example, is developed with a special focus on the easy applicability of the method for SMEs.

For this purpose, after analyzing the initial situation as well as the scientific questions, this thesis presents a three-step approach for modeling, simulation model generation as well as holistic and hybrid simulation of production systems in the beverage industry. At the beginning, the complex consumption structures of the different production areas of the brewery as well as the main consumers are revealed. The elaboration of the barriers which exist, especially for SMEs, to produce energy efficient provides the requirements for the application of approaches to increase energy efficiency. The approaches available in the scientific literature are presented, categorized, critically discussed and the scientific gap, the lack of a holistic method for forecasting the energy and media demand for complex production systems, is elaborated. For this purpose, in the first stage, a metamodel, which formally describes models, is developed as a standardized and generic framework for the representation of production systems, divided into the models: plant, process, article/recipe and production plan. The implementation of the metamodel in a user-friendly software allows easy modeling without pre-qualification of the user and opens up the method to wider application thus creating a broader fact base for further scientific developments. A standardized configuration file for the distribution of the model is presented and the software is validated by a systematic test and by use cases. Based on the configuration file, the simulation model is automatically generated in a simulation environment in the next stage. Furthermore, a generic and standardized data structure as well as tools based on this structure for the uniform and automatic determination of the required simulation parameters are presented. The simulation environment is extended by the integration of a production plan and the associated recipe- or article-specific simulation as well as by the simulation of batch-oriented production. Detailed validation is performed in both production areas of the brewery and simulation experiments are carried out. This shows that the method is able to map the energy and media demand of the brewery's production systems holistically and to forecast the demand of electrical and thermal energy within a deviation of about two percent in total. The final stage is the hybrid simultaneous simulation of the batch-oriented production method in the batch area and the discrete packaging and bottling area. This opens up far-reaching possibilities with regard to the holistic analysis of the dependencies and interrelationships of complex production operations by revealing optimization potentials, testing optimization measures and quantifying investments.

In summary, a metamodel-based hybrid simulation approach of production systems of the beverage industry regarding energy and media demand is presented. Its feasibility and suitability, especially for SMEs, could be demonstrated by the user-friendly implementation of the method as well as by simulation experiments. For future studies, the deepening of the method with regard to the integration of energy and media generation could enable further optimization potential as well as overcoming the barrier of data acquisition by directly connecting the production facilities to the method.

Zusammenfassung

Die Getränkeindustrie ist durch die steigenden Preise für Energie und Strom, sowie durch wirtschaftliche, ökologische, soziale und politische Bedingungen, wie die Verabschiedung der UN-Nachhaltigkeitsziele, besonders gefordert nachhaltig und effizient zu produzieren. Die energieintensive Produktion innerhalb der Brauerei, welche durch komplexe und hybride Prozessketten sowie einer Vielzahl an verschiedenen Maschinen gekennzeichnet ist, stellt ein gutes Beispiel für die Getränkeindustrie dar. Gerade für kleine und mittelständische Unternehmen (KMUs) bestehen spezifische Barrieren wie Zeit-, Kapital- und Knowhow-Mangel, um Potenziale zur Steigerung der Energieeffizienz zu identifizieren und entsprechende Maßnahmen zu ergreifen. IT-gestützte Ansätze können diese Barrieren überwinden und bieten den Entscheidungsträgern die Möglichkeit, zahlreiche Ansätze zu verfolgen und fundierte Entscheidungen zu treffen. Allerdings ist zurzeit keine Lösung, welche eine ganzheitliche Analyse und Prognose des Energie- und Medienbedarfs der hybriden Produktion der Getränkeindustrie ermöglicht und auch für die Anwendung in KMUs geeignet ist, beschrieben. Bisherige Ansätze konzentrieren sich bislang nur auf Teilbereiche sowie einzelne Aspekte und zeichnen sich durch eine hohe Komplexität aus.

In dieser Arbeit wurde eine Methode zur ganzheitlichen und hybriden Abbildung, Simulation und Prognose des Energie- und Medienbedarfs in der Getränkeindustrie, am Beispiel der Brauerei, mit besonderem Augenmerk auf der einfachen Anwendbarkeit der Methode für KMUs, entwickelt. Hierfür wird nach der Analyse der Ausgangssituation sowie der Anforderungen ein dreistufiger Ansatz zur Modellierung, Simulationsmodellerzeugung sowie zur ganzheitlichen und hybriden Simulation von Produktionssystemen der Getränkeindustrie präsentiert. Dabei werden zu Beginn die komplexen Verbrauchsstrukturen der unterschiedlichen Produktionsbereiche der Brauerei sowie die jeweiligen Hauptverbraucher aufgedeckt. Die Erarbeitung der Barrieren, welche vor allem für KMUs bestehen, um energieeffizient produzieren zu können liefert die Anforderungen an die Anwendung von Ansätzen zur Steigerung der Energieeffizienz. Die in der wissenschaftlichen Literatur verfügbaren Ansätze werden vorgestellt, kategorisiert, kritisch diskutiert und die wissenschaftliche Lücke, das Fehlen einer ganzheitlichen Methode zur Prognose des Energie- und Medienbedarfs, herausgearbeitet. In der ersten Stufe wurde ein Metamodell, welches Modelle formal beschreibt, als standardisierter und generischer Rahmen für die Darstellung von Produktionssystemen entwickelt, unterteilt in die Modelle: Anlage, Prozess, Artikel/Rezeptur und Produktionsplan. Die Implementierung des Metamodells in einer benutzerfreundlichen Software ermöglicht eine einfache Modellierung ohne Vorqualifikation des Anwenders und öffnet die Methode für eine breitere Anwendung, wodurch eine breitere Faktenbasis für weitere wissenschaftliche Entwicklungen geschaffen wird. Eine standardisierte Konfigurationsdatei für die Weitergabe des Modells wird präsentiert und die Software mithilfe eines systematischen Tests sowie anhand von Anwendungsfällen validiert. Ausgehend von der Konfigurationsdatei wird in der nächsten Stufe das Simulationsmodell in einer Simulationsumgebung automatisch generiert. Weiterhin wird eine generische und standardisierte Datenstruktur sowie Tools zur einheitlichen und automatischen Ermittlung der benötigten Simulationsparameter vorgestellt. Die Simulationsumgebung wird durch die Einbindung eines Produktionsplans und der damit zusammenhängenden rezept- bzw. artikelspezifischen Simulation sowie durch die Simulation der chargenorientierten Produktion erweitert. In beiden Produktionsbereichen der Brauerei erfolgt eine detaillierte Validierung und Simulationsexperimente werden durchgeführt. Die Ergebnisse zeigen, dass die Methode in der Lage ist den Energie- und Medienbedarf von Produktionssystemen der Brauerei ganzheitlich abzubilden und korrekt, mit einer Abweichung von insgesamt ca. zwei Prozent, zu prognostizieren. Die finale Stufe bildet die hybride Simulation der chargenorientierten Produktionsweise im Batch-Bereich sowie des diskret arbeitenden Verpackungs- und Abfüllbereiches zur gleichen Laufzeit. Dies eröffnet weitreichende Möglichkeiten hinsichtlich der ganzheitlichen Analyse der Abhängigkeiten und Zusammenhänge von komplexen Produktionsbetrieben durch die Aufdeckung von Optimierungspotentialen, dem Testen von Maßnahmen und der Quantifizierung von Investitionen. Zusammenfassend wird ein metamodellbasierender, hybrider Simulationsansatz von Produktionssystemen der Getränkeindustrie hinsichtlich des Energie- und Medienbedarfs präsentiert. Dessen Durchführbarkeit und Praxistauglichkeit, wird durch die anwenderfreundliche Umsetzung der Methode sowie durch Simulationsexperimente gezeigt. Für zukünftige Studien könnte die Vertiefung der Methode hinsichtlich der Einbindung der Energie- und Medienerzeugung weiteres Optimierungspotential ermöglichen und durch die direkte Anbindung der Produktionseinrichtungen an die Methode die Hindernisse der Datenerfassung überwunden werden.

1 Introduction

The adoption of the UN Sustainable Development Goals obliges member states to integrate them into national targets. In view of climate change and the resulting environmental challenges, as well as the economic progress, ambitious goals have been set until 2030 [1]. Furthermore, companies are currently confronted with rising prices for energy and electricity and are thus forced to produce in a particularly sustainable manner and to save energy in order to be able to continue to exist on the market and to meet the requirements of customers [2]. Global industrial energy consumption is expected to increase by 29% from 2020 levels by 2040 [3]. Germany is the world's seventh largest consumer of primary energy, with German industry playing a major role [4]. The energy demand of the food and feed industry ranks sixth [5], where the two economic indicators "Production of food and feed" and "Beverage production" account for around 16 % of the total German industrial energy demand of the manufacturing industry [6]. The food and animal feed industry leads the way in investments to increase energy efficiency [7] as it ranks third with the highest energy expenditures [8]. In 2020, the German food industry generated sales of EUR 164 billion [9], while the beverage industry accounts for 8% of sales [10]. This shows the importance of reducing production costs, and not only for German beverage producers, in order to remain competitive. Beer production is one of the most energy-intensive production processes in the food industry and is characterized by numerous heating and cooling processes in the brewhouse depending on biological and chemical influences as well as the use of numerous pumps and motors for material movement, and complex packaging and filling processes [11–14]. In addition, the beverage industry is challenged by high market dynamics, which require a large product range and extremely flexible production as well as high product quality in combination with a cost-effective production. The energy saving potentials are manifold and can be uncovered and addressed in all areas as well as facets [12]. Energy-efficient production can sustainably reduce costs and increase competitiveness [15, 16]. Therefore, precise knowledge of the processes is essential [17]. The world's major brewing companies are ambitious about their sustainability, proclaiming goals such as CO_2 neutrality and halving water consumption by 2040 [18–20]. However, sustainable and efficient production also concerns SMEs. 90% of German breweries are SMEs with an annual production of less than 50,000 hl [21]. They are, in particular, required to produce sustainably and energy-efficiently to withstand the enormous competitive pressure [22]. However, SMEs of the beverage industry are confronted with insurmountable barriers such as lack of capital and human resources as well as insufficient data and information to achieve efficient and sustainable production [23, 24]. Furthermore, they often lack the time and knowledge to identify and implement suitable energy efficiency measures [25]. IT-supported analysis and prediction methods, such as simulation, represent an opportunity to uncover optimization potential and can thus contribute to energy efficiency and sustainability [26, 27]. The advantages of simulation lie in the representation of complex processes and interrelationships as well as in experimental analysis through the adaptation of models without interrupting or influencing ongoing production. In addition, simulation can be used for holistic forecasting of complex production systems [28, 29]. However, simulation studies are usually associated with high costs and require a high level of expertise, especially for the modeling and creation of complex simulation models. In addition, a comprehensive database, which is necessary for the determination of reliable simulation parameters, is essential for dependable simulation results [30].

The ability to quickly and easily analyze and simulate production systems in the beverage industry in terms of their energy and media demand would represent added value for the entire beverage industry. This applies in particular to SMEs, which would otherwise not be able, or only at great expense, to carry out simulations and thus forecasts of the energy and media requirements of their production systems in order to achieve sustainable, energy- and media-efficient production. Previous approaches also focused only on sub-areas and selected energy and media types and require specific knowledge in the area of modeling and simulation. In the following sections, the essential basics of modeling and simulation of production systems in the beverage industry will be discussed and the most important previous approaches will be summarized. This provides the necessary basis for the understanding of the present work. The objective of this work is presented and the scientific questions addressed by this work are outlined.

1.1 Modeling

A system describes a set of elements (E) which are separated from their environment and are connected with each other [31]. The system is characterized by the definition of boundaries with respect to its environment as well as by interfaces describing interactions with this environment. Interactions of input (I) and output (O) variables can be described, which include, for example, material, energy and media as well as information. Within the system, system elements, which can adopt system states (S), can be defined up to the required level of detail [32]. State transitions of the elements result from continuous or discrete changes of state variables due to processes occurring in the system. In addition, individual elements contain a flow structure, which are described by specific rules regarding the states [33].

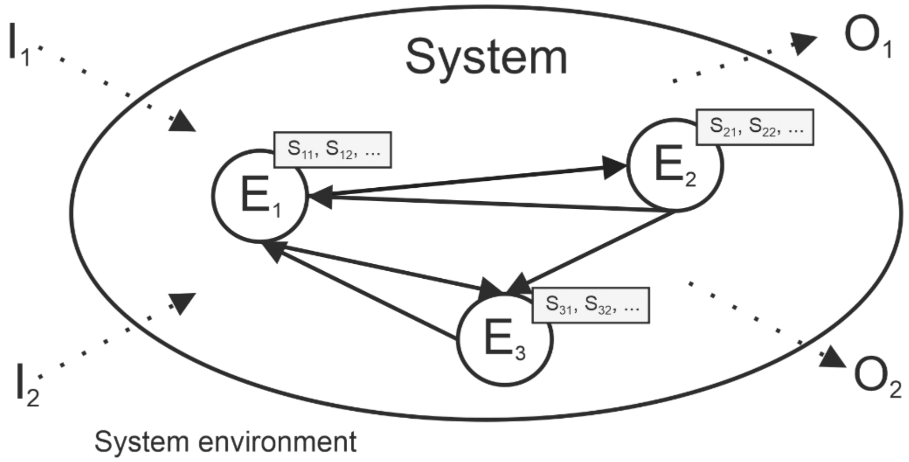

Figure 1: Visualization of the system concept (adapted from [32])

If the aim is to analyze a system in terms of its performance and functionality, this can be represented in a model. The examination of a system is only conditionally purposeful, since it can be a fictitious system or interventions in the system are not possible without restrictions. The model remedies this by representing the system in an abstracted manner with clear system boundaries and with all properties and parameters relevant for the model purpose [32]. The level of detail (granularity) is a measure of the accuracy with which a system is represented in a model [33].

Complex systems can be represented in models in a simplified manner by examining and representing selected objects in a purpose-oriented manner as part of the overall design process [32, 34]. Essential for the simplification of a real system is the prior definition of the purpose of the model, which is why the system optimization should be done in terms of system structure, behavior and function [35]. A too high a level of detail can be counterproductive, as the models become more complex and the level of detail may not be necessary for the goal of the study. Furthermore, this also leads to increased effort and thus costs [33].

Metamodels represent higher-level models for the formal and conceptual description of other model concepts and thus comprise the essential elements of the models to be described. A metamodel describes models in a generic way for specific research purposes, standardizes them and is therefore particularly suitable for the interpretation and analysis of highly complex models [36]. Figure 2 shows schematically how higher-level models (M2 to M1; M1 to M0) in a specific language (S1) can be reformulated into another model (M1, M0) in another language (S0) and thus describe it. A metamodel can therefore be compared to a module kit for models, in which the interfaces of the individual elements are also described [37]

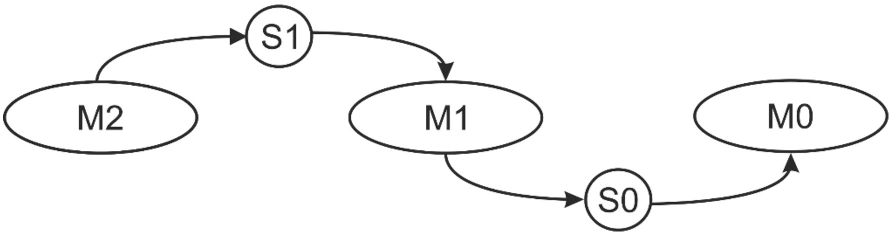

Figure 2: Relationship between metamodel and model [38]

The UML (Unified Modeling Language) modeling language of the OMG (Object Management Group) is often used to describe a metamodel with the aid of class diagrams. The advantage lies in the standardized definition and representation of objects including all attributes as well as relationships and dependencies. In particular, classes consisting of structurally identical objects guarantee the unambiguous model specification of the model components within a delimited system. Another advantage of using the graphical and formal notation of UML is the transformation of the complex structure into other languages, such as XSD (XML Schema Definition), which excels for the formal description of XML (Extensible Markup Language) files [39]. XML is suitable as a language for the simple and textual description of structures and dependencies as well as their data contents and is capable of a platform-independent exchange of information and can therefore be used for the transfer to systems such as simulation environments [40]. The transformations between the individual (meta-) models with their specific languages can be realized automatically via transformation patterns [41, 42].

The knowledge of which system is involved is essential for the model creation. Systems can be investigated either on the basis of models that represent the system on a laboratory scale, for example, or on the basis of mathematical models. The former does not seem to be appropriate for holistic investigations of complex production systems in the beverage industry. Analytical solutions of complex models can usually only be solved with enormous computing power. This is why the investigation by means of simulation is recommended [43–45].

In general, a distinction can be made between different types of mathematical models, which are divided into static and dynamic models. In contrast to static models, dynamic models are characterized by their behavior with respect to the progressing time. Furthermore, dynamic models can be described as continuous or discrete in terms of time and state. In discrete-time models, the component time is divided into time points with equidistant intervals. The expression in the mapping of state transitions can be due to coincidences (i.e. stochastic models). In deterministic models, however, the subsequent states are unique. When different types of models are combined, they are referred to as combined models. The conversion of the respective model into a computer model enables the later IT-supported analysis of the model [32].

The beverage industry in particular is characterized by the combination of different models. The production of the beverages follows the batch-oriented production method and the filling and packaging of these is carried out according to the discrete production [46, 47].

For a practical application or implementation of the modeling, numerous framework conditions have to be considered in order to obtain a sound model later on. Therefore, in a first modeling step, it is necessary to check which system elements and properties are relevant and therefore of interest for the purpose of the model, which results from the previously defined problem [32]. A further step involves the implementation of the model in a suitable software environment. On the one hand, programming languages can be used for textual modeling, and on the other hand, graphical modeling can be used within a simulation environment. Table 1 illustrates the advantages and disadvantages of the different creation of models of production systems [33].

Table 1: Advantages and disadvantages of graphical and textual creation of computerized models of production systems [33]

	Programming language	Simulation incl. modeling
Pros	• Great flexibility in terms of application and questioning	• Required simulator components as a package • Graphical-interactive model creation and modification • No programming necessary • Direct experimentation • User-friendly • Little error-prone
Cons	• High effort • Error prone • Expert knowledge necessary	• Often specific application areas • Less flexibility

In combination with the previous formal description of a model through, for example, the use of metamodels, these approaches can also be used to create suitable modeling environments. This is referred to as MSD (Model-Driven Software Development) approaches, since abstract representations of the aspects of the requirements are necessary in this case. Depending on the application purpose, mathematical or visual modeling is useful. Especially for the representation of complex workflows and processes, graphical modeling is usually appropriate for several reasons [39].

MSD consists of the three components: model, notation and generation of executable code [39]. For the modeling of production systems in the beverage industry, tools are sometimes already available [48–50]. However, these are not suitable with regard to a holistic investigation [51], which is why the development of specific modeling solutions is recommended.

For modeling, the selection of a suitable modeling philosophy, such as a petri net-oriented or building block-oriented approach, is also crucial. Building block-oriented modeling is performed using predefined standard elements [33], which can be adapted by the user according to the intended use. Within this modeling approach, it is possible to fall back on already existing modeling standards and their notation [39]. Examples include Business Process Model and Notation (BPMN) [52] as well as standards for subdividing production systems, such as American National Standards Institute (ANSI)

/ International Society of Automation (ISA)-88 [53]. This is to ensure that the applied modeling language explains itself through language concepts, models are consistent and uniformly structured, and semantically correct [39].

Finally, it must be ensured that the goals and application areas formulated at the beginning of the modeling process are achieved. Especially with regard to the adequate representation of a production system in terms of the purpose of the model, validation is essential [32, 54].

1.2 Simulation

According to Verein Deutscher Ingenieure (VDI) Guideline 3633 for Simulation of systems in materials handling, logistics and production, the term simulation is understood to mean "*the representation of a system with its dynamic processes in an experimentable model to reach findings which are transferable to reality*". Simulation can be applied along the entire development phases: planning, implementation and operation phase of processes or production systems and its procedure for application is clearly described [33]. Simulation is thus an essential part of process engineering [54] and is used for the development, optimization and validation of processes [55]. In addition, important principles for the execution of simulation studies are described. It is essential that the simulation is carried out before the investment is made. Furthermore, a prior definition of the objective as well as an estimation of the expenditure are to be carried out in advance and in this course all analytical methods are to be exhausted. It is essential that simulation is not a substitute for planning and that the mapping accuracy should not be chosen as large as possible, otherwise the purpose of the investigation is not met. Regarding the results of simulation studies, it is considered that they are directly dependent on the database as well as on the processing persons. Nevertheless, simulation allows far-reaching options, such as the investigation of real systems, which do not yet exist, without directly influencing them and their production. Multiple variants of different extent can be tested without great effort and the system behavior can be determined over long periods of time. Furthermore, specific phases such as start-up processes, transient phase and transitions between operating states can be investigated [33].

The simulative concept of optimization specifies that a process is a dynamic system equipped with a process logic [54]. Exclusively suitable for the study of complex systems is computer simulation, in which modeling leads to a simulation model that can be run as a computer program [32].

Dynamic production systems are characterized by their time dependence due to the change of states. Several methods have been described for simulation in terms of progressive simulation time [43].

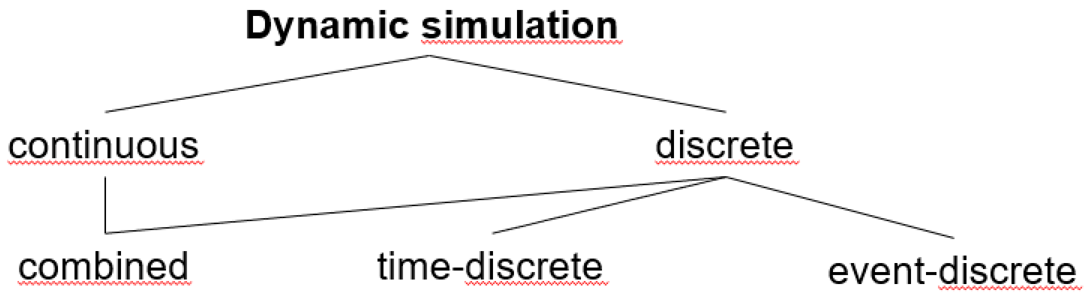

Figure 3: Overview of the methods of dynamic simulation [32]

Figure 3 shows within the dynamic simulation the continuous, discrete and combined simulation. The former is defined by a continuous time set and time progress as well as continuous state transitions and describes systems mostly by differential equations, mathematical relations or empirical models. Since continuous simulation is not applied in this thesis, it will not be discussed in detail. On the one hand, the discrete simulation can be divided into an event-oriented simulation, in which the simulation time is increased when an event occurs. In this case, the previously defined list of occurrence times of the future events and thus of the state variables is updated. This procedure is repeated until a termination condition is met. Inactive time periods are skipped in the simulation. On the other hand, time-controlled simulation describes the progression of the simulation by a fixed constant equidistant step size, where the system is observed in a corresponding time interval. State changes within a time interval are not explicitly considered and are only performed when the next point in time is reached. Depending on the choice of the time interval, the simulation is more or less computationally intensive [32, 43, 54]. The combined simulation is characterized by the combination of the continuous and discrete simulation. In this way, the continuous change of the system between events or fixed times of the discrete simulation can be described [43, 56].

A prerequisite for carrying out simulation studies are executable simulation models, which represent the dynamic relationships of the system under investigation. In this context, the modeling of time, the stochasticity of the occurrence of events as well as the automatic execution of the simulation are of essential interest [32]. Simulation studies are generally divided into three phases: preparation, execution, and evaluation. The first phase includes the goal formulation of the simulation study, considering the analysis of the problem and the costs, including the verification of simulation worthiness. Subsequently, data of the system to be investigated are collected and a model is created on the basis of this data. This phase comprises by far the largest scope and is time and cost intensive [57]. One approach to solving this problem can be the automatic generation of simulation models. Here, the basis for a simulation model is created from external data sources by means of various interfaces as well as acquisition and modeling methods. One possibility can be the statistical determination of parameters as well as the manual collection of data by user input [58, 59]. A suitable transfer of the entire structures as well as information can be realized via an XML file [60, 61]. In this case, the creation of the simulation model itself is the task of the simulation environment planned for use, which must reformulate the structure as well as all parameters, build and initialize the simulation model, and continuously retrieve the corresponding parameter sets [59]. After the simulation has been completed, the results can be evaluated and interpreted. Conclusions can be drawn on the basis of the results and appropriate measures can be initiated.

Verification and validation play an essential role in the execution of simulation studies. These ensure in each of the phases that erroneous statements of the simulation experiments are reduced and thus wrong decisions can be avoided. Verification ensures the transformation of a model from one type of representation to another and checks it for validity. Thus, specifically, the transformation of a conceptual model into a simulatable model can be verified. Validation ensures that the model correctly reflects the behavior of the original system for the specific application purpose. Validation occurs at each step of model creation and is the basis for using a model or simulation method to create simulation experiments with reliable and reproducible results [62].

1.3 Selected scientific literature for the modeling and simulation of production systems in the beverage industry

Approaches for modeling and simulating the energy and media requirements of production systems in the beverage industry have already been described in the scientific literature. The most relevant publications for this thesis will be briefly presented and the resulting scientific gaps, which the present thesis tries to close, will be elaborated. The scientific literature research is listed in the corresponding chapters of the publications comprising this thesis. Furthermore, these publications contain a detailed description of the processes that take place in the brewery, the equipment and machinery that occur, their consumption structure and behavior, and the subdivision of the brewery as a production system according to ANSI/ISA-88 [53]. The essential basis for the modeling and simulation of energy and media demand is the understanding of the different consumption behavior and operation of the batch-oriented and discrete production area. Muster-Slawitsch *et al.* [51] and Mignon and Hermia [63] describe the consumption behavior in the batch area of the brewery as depending on the currently running process. According to Osterroth *et al.* [64], in the area of discrete working packaging or filling of beverages, the consumption behavior depends on the currently applied operating state according to [65] of the respective machine. In their work, a time-dependent behavior within the individual operating states is described in more detail [64, 66].

An approach for modeling production systems of the beverage industry with regard to the automatic generation of Manufacturing Execution Systems (MES) is described by Weissenberger *et al.* [67]. Incorporating already existing standards regarding the description of production systems as well as the modeling language, the model generation is based on the independent mapping of the production facilities as well as the processes. The concrete implementation and application to the brewery is shown by Chen *et al.* [68].

Table 2 shows an overview of scientific publications in the field of forecasting methods of energy and media demand in the beverage industry. The publications are categorized with regard to the methods used, the energy and media type, and the areas of application. Based on this, the most important publications for this work are discussed. More detailed descriptions of the other methods can be found in Publication I (see section 2.1).

Table 2: Categorized overview of scientific literature approaches to forecasting methods in the beverage industry with regard to energy and media demand (adapted from [69]); (x) ~ partly

Publication	**Methods**				**Energy and media type**			**Area of application**			
	Pinch	Simulation	Mathematical	Reference nets	Thermal	Electrical	Water	Brewhouse	Cellar/Filtration	Packaging	Utilities
Mignon and Hermia [63]		x						x			
Mignon and Hermia [70]		x						x			
Zhelev and Zheleva [71, 72]	x						x				x
Dilay *et al.* [73]			x			x				x	
Johansson *et al.* [74]		x				x		(x)	x	x	
Gahbauer *et al.* [75]	x					x		x	x	x	x
Dumbliauskaite *et al.* [76])	x					x		x	x		x
Tokos *et al.* [77]			x			x		x			x
Marty *et al.* [78]	x							x		x	x
Muster-Slawitsch *et al.* [79]	x	(x)						x	x	x	
Nagel [80]		(x)		x				x			
Bai *et al.* [81]			x			x	x	x	x		x
Sturm *et al.* [82]		x				x		x	x		x
Forster [83]		x				x				x	
Muster-Slawitsch *et al.* [84]	x				x			x		x	x
Muster-Slawitsch *et al.* [51]			x		x	x		x	x		
Marchini *et al.* [85]		x					x		(x)	(x)	
Hubert *et al.* [86]		(x)		x			x	x	x	x	x
Hubert *et al.* [87]		(x)		x			x			x	
Pettigrew *et al.* [88]		(x)		x	x	x	x				x
Müller [89]	x	x			x	x		x	x	x	x
Hubert *et al.* [90]		(x)		x	x			x	x		
Hubert *et al.* [91]		(x)		x	x		x	x	x	x	
Tibasiima and Okullo [92]	x				x			x	x		x
Osterroth *et al.* [64]		x				x				x	
Hubert [93]		(x)		x	x	x	x	x	x	x	

Forecasting methods such as pinch analyses and mathematical approaches are not suitable for the approach presented in this work as they usually target sub-areas of production facilities and are limited to single energy and media types. For example, pinch analysis usually describes only the optimization of heat flows and the saving of thermal energy. Mathematical models are also only partially able to represent the complex interrelationships of production systems in the beverage industry with sufficient accuracy and to forecast the energy and media demand. Therefore, the following section focuses on approaches for modeling and simulating production systems in terms of their energy and media demand.

The first concrete application for modeling and simulation within the batch area of the brewery is described by Mignon and Hermia [63]. With the help of the simulation software BATCHES [49], the batch and semi-continuous processes within the brewhouse of the brewery are mapped and divided into the units, recipes and production plans according to the ANSI/ISA-88 standard. The object of investigation of the simulation was carried out in several works on the reduction of the energy and media demand by the influence of the plant composition [63], the production plan [94] as well as the reduction of peak loads [70]. Another approach is described by Muster-Slawitsch *et al.* [51] by modeling the equipment, processes, energy flows as well as a production schedule of the brewery by simultaneous non-linear equations using the Engineering Equation Solver (EES) software. By changing the process parameters, an attempt is made to affect the energy flows in the brewhouse and thus reduce the peak thermal energy demand as well as the cooling load. The modeling and simulation of reference nets, a further development of petri nets, and their implementation in a Java environment is described by Hubert *et al.* [86] as another main approach in the literature. Here, the reduction of the brewery's water demand is investigated. The modeling and simulation of water demand as well as wastewater quality by combining the continuous and discrete simulation methods for a beverage bottling plant is applied in another publication [87]. Furthermore, based on reference nets, a holistic approach for the investigation of the overall electrical energy demand of the production facilities is presented [91]. In addition to other works on the application of reference nets [88, 90], Hubert [93] comprehensively describes the application of the method in numerous areas of the brewery in his dissertation. Different factors, such as the quality of the raw materials and the process quality, but also the electrical energy demand of the Cleaning in Place (CIP) system are investigated. With the inclusion of production schedules, the consumption structures of electrical and thermal energy as well as the demand for fresh water and the production of waste water are simulated.

In the area of filling and packaging of beverages, Osterroth *et al.* [64] deals with the simulation of the electrical energy demand of the individual aggregates based on the approach already presented using Matlab-Stateflow. A holistic approach developed in Plant Simulation for building block-based modeling of beverage bottling plants is presented by Forster [83]. In the discrete-event simulation, the machines are examined with their state-dependent consumption behavior.

In general, the following conclusions can be drawn regarding the different approaches to modeling and simulation of energy and media demand in the beverage industry described in the literature. Currently, there is no generic and holistic modeling approach described for the representation of an entire production plant of the beverage industry with its different plants, processes as well as recipes and articles including a production plan. The advantage of a metamodel and a standardized modeling approach would be the generic definition of the data and information needed for predictive models. These are not described so far. Furthermore, this represents a good basis for the derivation of measurement concepts and data acquisition.

Furthermore, the complexity of certain modeling approaches, such as the description by equations or also by means of reference nets, represents a significant challenge in the practical application of the methods. The existing methods require a special degree of specific know-how as well as expert experience in the field of modeling and simulation and are therefore only suitable for SMEs to a very limited extent. Overcoming this barrier would increase access to such a method, making it available to stakeholders. Increased application will expand the knowledge and database in this field and possible further scientific questions can be uncovered. Implementations of the methods in user-friendly environments are not available. This is urgently required in order to be able to map above all a holistic method for the creation of simulation models, which includes all necessary data.

Regarding the data needed for a reliable statement of simulation studies, there is currently no standardized procedure for the collection as well as for the processing of these. Furthermore, no standardized approach for the determination of the required simulation parameters is described. The scope of the available database is for the most part severely limited in the published approaches. This also leads to a mostly limited or non-existent validation of the approaches with real data. Validation is another important point, which is only applied to a very limited extent in existing approaches. However, this represents an essential point to ensure the functionality of the whole method and to guarantee reliable statements for later simulation studies.

The approaches described in the literature have in common that not all production areas of the brewery are represented and mostly only a reference to partial areas takes place. There is no exact definition of a required level of detail of the modeling for the simulation of the holistic production. In addition, none of the approaches includes all relevant energy and media types, such as electrical and thermal energy as well as water, CO_2, and compressed air.

The mapping and simulation of a production plan is only carried out in a small part of the approaches. This is accompanied by the consideration of different recipes or articles, which in turn means different parameter sets. This has a direct effect on the corresponding behavior of the plants and machines as well as their consumption values. A simultaneous simulation of the differently operating production areas (batchwise and discrete) has not been described for the beverage industry so far. This is the prerequisite for a holistic consideration of production systems with regard to their energy and media demand, as the complex interrelationships and dependencies must be represented.

The creation of simulation models also plays an important role, since most of the time of simulation studies is spent on this. None of the approaches in the scientific literature addresses this topic and offers a solution, for example the automatic generation of simulation models.

1.4 Motivation and objective

In summary, a comprehensive method consisting of a generic and context-free modeling approach based on a metamodel in combination with an automatic generation of simulation models can be a solution for the holistic representation and prediction of the energy and media demand of production systems in the beverage industry. The hybrid simulation of batch-oriented production in the batch area of the brewery with discrete production in the beverage filling -/packaging area is of essential importance. With the inclusion of a production plan, it becomes possible to achieve a holistic simulation with all its interrelationships and dependencies. An implementation of the metamodel in a user-friendly software solution, which does not require any special prior knowledge for operation, in combination with the automatic generation of simulation models based on it, would open up the method to broader application and creates a broader fact base for further scientific developments. Furthermore, the method would represent a considerable added value for SMEs. Since the German brewing landscape is characterized by SMEs and they face particular barriers to increasing the energy efficiency of their production, this, as well as the definition of a standardized data structure based on which the required simulation parameters can be determined, could contribute to achieving efficient and sustainable production. Based on the simulation results, unexploited potentials for increasing energy efficiency, optimization solutions and innovative scenarios for energy supply can be found and defined, and investment decisions can be backed up by valid data.

The aim of this thesis is the development of a modeling approach, the automatic generation of simulation models and the holistic and hybrid simulation of production systems of the beverage industry for the prediction of energy and media demand, with special focus on the easy applicability of the method for SMEs. The scientific questions to be answered by this approach are defined as follows:

- **Scientific Question 1 (SQ1): Generic metamodel for the modeling of complex hybrid production systems**

The challenge on an approach for the holistic and hybrid mapping of complex production systems in the beverage industry with regard to their energy and media demand is that every possible production system must be able to be mapped. A generic metamodel could be used to describe the complex interrelationships and dependencies of the existing plants, processes, recipes and articles as well as the production plan, in a context-free manner. Flexibility of the metamodel with respect to granularity may be of essential interest, so that, on the one hand, individual units can be mapped in the required depth of detail with regard to their real consumption behavior. On the other hand, entire systems could be modelled with sufficient accuracy, e.g. with a focus on only one type of energy. For this purpose, a verification of the modeling solution with suitable methods and on real plant complexes is essential. This should already result in the information and data required for later modeling and simulation. Additional features of the metamodel could be the consideration of already existing standardizations and modeling languages. This would simplify a later implementation of the metamodel and enable a broad application of the method.

- **Scientific Question 2 (SQ2): Implementation of the metamodel in a software to enable accessibility to the method**

The scientific question lies on the one hand in the implementation of the hybrid, holistic and generic metamodeling approach and on the other hand in the solution finding which functions a software has to provide in order to ensure a later broad application. The developed generic metamodel should be implemented in a software solution in order to represent the context-free modeling of production systems divided in their components on one side. On the other side, the interrelationships and dependencies of the metamodel should be implemented in the software solution with respect to their functionality. For this purpose, the modeling within the individual modeling columns should be based on suitable modeling languages or mapping types that fulfill the required functionality. A basic component library based on building blocks, which represents the majority of the plants and processes occurring in the beverage industry, could be a practical solution. Nevertheless, the functionality of the modeling solution should be open to extensions and specific adaptations to be able to represent innovations and the production systems of other industries. In addition, the software solution should cover all functions required for practical work with it, so that the method can be widely applied and thus new facts can be created for further research in this field. For this purpose, verification of the modeling solution with appropriate procedures is essential.

- **Scientific Question 3 (SQ3): Development of a data structure, determination of simulation parameters and usability of the approach**

In order to provide a basis for the information and parameters needed for a simulation, a consistent approach should be developed. A generic data structure for hybrid production systems with their different energy and media consumption behavior should make this possible and could present the data in a uniform and standardized way and show their interrelationships. The data structure should serve equally for the raw data as well as for the result data of the simulation. Tools based on the structure could enable a standardized and uniform determination of the simulation parameters and could also take over the evaluation of the simulation result data. These developments as well as further implementations along the entire method should be validated in order to ensure the usability and applicability of the method and thus the application without special knowledge as well as to guarantee the validity and function of the simulation models. Thus, the approach can be made accessible through further use and open up further research fields.

- **Scientific Question 4 (SQ4): Development of automatic simulation model generation**

An automatic generation of prognosis-capable holistic simulation models in any suitable simulation environment represents one of the essential scientific questions. This would enable the generic application of simulation of production systems on the basis of standardized models. Furthermore, the application of simulation would be simplified and thus barriers would be reduced. The generation should be based on the models created in the modeling solution and without further required settings and parameterizations to reduce the effort normally required for simulation studies. For this, a solution must be found to reformulate the structures and individual modeling columns of any simulation environment. A particular challenge is posed by the differently operating production areas of the plants in the beverage industry as well as changing parameter sets of the elements in the simulation environment due to the required implementation of the production plan and the associated different recipes and articles.

- **Scientific Question 5 (SQ5): Development of holistic hybrid simulation**

The simulation environment should be able to represent a holistic simulation of production plants and systems in the beverage industry. Of special importance is the representation and hybrid simulation of the two differently working production areas of the brewery, which at the same time represents the scientific question as well as essential novelty of this work. Another challenge is the implementation of a production plan and the associated recipe and product specificity of the simulation parameters in the approach to be developed. In addition, it should be possible to simulate any number of areas at the same runtime for a holistic view of an entire production plant in order to map the interrelationships and dependencies. To validate the solution to this question, the resulting method must be validated and tested with use cases.

This thesis is structured as follows:

1. Literature study for state of art:
   Analysis and Prediction Methods for Energy Efficiency and Media Demand in the Beverage Industry

2. Development of a metamodel and software for a holistic model of production plants:
   A metamodeling approach for the simulation of energy and media demand for the brewing industry

3. Automatic model generation and simulation of the discrete bottling area of the brewery:
   Simulation of Energy and Media Demand of Beverage Bottling Plants by Automatic Model Generation

4. Simulation of the batch-oriented production of the brewery and holistic hybrid simulation:
   Simulation of Energy and Media Demand of Batch-Oriented Production Systems in the Beverage Industry

2 Results – Thesis Publications

2.1 Publication I – Literature study for the state of art

Bär, Raik; Voigt, Tobias. **Analysis and Prediction Methods for Energy Efficiency and Media Demand in the Beverage Industry**. Food Eng. Rev. 2019, 11, 200–217; DOI: 10.1007/s12393-019-09195-y

The energy-intensive production of beverages poses an economic, ecological and social challenge to the beverage industry. High costs for energy as well as the increasing competitive pressure force companies to urgently act in order to survive in the market. Especially for SMEs there are specific barriers like lack of time, capital and know-how to identify potentials to increase energy efficiency and to take appropriate measures. IT-based approaches can overcome these barriers and provide an opportunity for decision makers to pursue numerous approaches and make sound decisions. In this literature work the existing barriers to energy efficiency in the beverage industry, especially for SMEs, are presented. A detailed insight is given into the complex consumption structure within the various production areas of the brewery as an example for the beverage industry and its main consumers are identified. Based on this, the approaches described in the scientific literature for optimizing energy and media efficiency within the beverage industry are categorized and described, and summarized in terms of the method used and the areas of application. It turns out that no tools or approaches are yet available that allow for simple, holistic analysis and prediction. The critical comparison of the different approaches makes it clear that simulation could enable a holistic analysis of energy and media demand of the brewery. Since the data basis is mostly insufficient and simulation requires expert knowledge, a novel modeling and simulation approach is proposed. An easy-to-use and context-free modeling environment should enable the generation of a simulation model in any simulation environment, with limited expertise or effort and help to overcome the barriers of SME.

Contributions of the doctoral candidate (CRediT):

Conceptualization; methodology; formal analysis; investigation; resources; data curation; writing - original draft preparation; visualization;

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Analysis and Prediction Methods for Energy Efficiency and Media Demand in the Beverage Industry

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Abstract
Since the production of food and beverages is energy-intensive, the political, economic, ecologic and social conditions are posing a challenge to the manufacturing industry. Small- and medium-sized companies in particular lack the time and knowledge to identify and implement suitable energy efficiency measures. With the help of computer-aided solutions, decision-makers can pursue numerous approaches and make well-founded decisions. The aim of this review is to summarise and critically discuss current analysis and prediction methods concerning energy and media consumption in the beverage industry. To date, there have been no tools or approaches available that permit a simple, holistic analysis and prediction. Breweries serve as a good example for the beverage industry due to numerous and various complex processes. To identify energy-saving potential, the main consumers and consumption structures within the brewery are presented. Current approaches such as simulations, pinch analyses, benchmarks and real-time operating systems are briefly explained, and the relevant publications related to the beverage industry described and categorised. The critical comparison of the different approaches clearly shows that simulation enables a holistic analysis and prediction of energy and media consumption in the brewery. Since the data basis is mostly insufficient and this method requires expert knowledge, we propose a holistic modelling and simulation approach. An easy-to-use and context-free modelling environment should enable the generation of a simulation model, with limited expertise or effort.

Keywords Beverage industry · Energy · Media · Efficiency · Consumption · Prediction

Introduction

Global industrial energy consumption will increase by 25% to 737 billion BTU by 2040 [1, 2]. German industry plays a major role in primary energy consumption and is the seventh-largest consumer of energy after China, the USA, India, Russia, Japan and Canada [3]. The energy consumption of the two economic indicators "Production of food and feed" and "Beverage production" was 236.7 million GJ in Germany in 2016, which corresponds to 17.2% of the total German industrial energy demand of the manufacturing industry (4 million TJ). The energy sources are almost exclusively natural gas and electricity. The share of renewable energy is approx. 1.1% [4].

As the production of food and beverages is energy-intensive, the political, economic, ecologic and social conditions are posing a challenge to the manufacturing industry [5, 6]. The opening up of international markets and the associated globalisation are steadily increasing the competitive pressure on companies. Energy-efficient production can sustainably reduce costs and increase competitiveness [7, 8]. Improving energy efficiency is, therefore, an important factor, not only in terms of climate change.

In 2017, the food industry generated sales of EUR 158.46 million [9]. In Germany, the beverage industry accounts for 13.3% of the food industry's turnover, which corresponds to a total of EUR 21.1 million [10]. The production of beer (37.2%), soft drinks and mineral water (the two of which make up 38.9%) is the mainstay of sales in the beverage industry [11]. Consumers spending on alcoholic and non-alcoholic beverages by private households in Germany has increased by 25% since 2000 to around EUR 43.72 billion in 2017 [12, 13]. This development shows the importance of reducing the production costs in order for (not only) German beverage manufacturers to remain competitive. The beverage

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industry is somewhat characterised by complex production in terms of the processes and machinery required. Due to numerous heating and cooling processes, the brewing process is one of the most energy-rich production processes in the food industry [5, 14, 15]. The brewing process can also be subdivided into two sub-areas with different properties. The beer production area follows a batch-oriented operating mode with a time horizon of several weeks, whereas the packaging area is characterised by discrete production and short delivery times. This complex production process is a suitable example for the beverage industry. Measures to increase energy efficiency and energy management can be illustrated using this example. There are numerous potential energy savings, including factors such as improved plant utilisation, heat recovery, cost-saving measures in the areas of refrigeration, heating technology and compressed air as well as the use of cogeneration [14]. Small- and medium-sized companies in particular lack the time and knowledge to identify and implement suitable energy efficiency measures [16]. IT-supported analysis and prediction methods can help here. Therefore, this review is intended to summarise and critically discuss current publications on the topic of analysis and prediction methods concerning energy and media consumption in the beverage industry. To date, there have been no tools or approaches available that permit a simple, holistic analysis and prediction of energy and media consumption. Therefore, the challenges for companies to work energy-efficiently—as well as the main consumers and consumption structures in the brewery—will be addressed at the outset. In the central part of this paper, the publications are categorised and thematically sorted. Subsequently, the methods will be critically discussed with regard to ease of use and a holistic, comprehensive approach. Finally, requirements for solving this scientific gap are presented.

Barriers to Energy Efficiency in the Beverage Industry

There are numerous barriers for companies to implement systems to manage or optimise their energy and media consumption. According to the United Nations Industrial Development Organisation (UNIDO) [17], the main barriers are as follows:

Lack of Capital and Capacity

At first, the technical and financial risks of investments in energy efficiency are higher than other investments. Furthermore, a barrier to energy-efficient work in companies is the hidden costs, which are difficult to estimate in advance. Energy efficiency investments are often prevented due to insufficient capital and the difficulty in procuring the necessary funds [17]. Trianni et al. conclude in their study for the European market that the main reasons for what has to date been a moderate interest from companies in energy-saving measures are reduced to two main problems. For small and medium enterprises, in particular, a lack of capacity and resources such as investment capital continues to be the main reason for a low level of commitment in the energy sector [18].

Imperfect Know-How and Organisation

However, Trianni et al. state that the most significant and most common barrier for small and large enterprises is the responsibility of entrepreneurs who want to ensure the operation and continuity of production, while adopting measures to improve energy efficiency [18]. Opportunities in terms of the implementation of energy efficiency measures and methods are also present due to the lack of allocation of responsibilities in an enterprise [17]. Fleiter et al. stated that the understanding for measures to increase energy efficiency can only be enhanced if the measures are classified. Due to the diversity of innovations and the objectives of the measures and methods, this is difficult to implement for companies [19]. Furthermore, the uncertainty about the effects of the implemented technologies on the existing process creates scepticism about possible savings with regard to energy use. A low willingness to invest in the energy sector reinforces this [16]. Kubule et al. underpin these statements. In a case study, they compared the specific energy consumption of an SME with literature values. The differences can be described using technological and non-technological factors. The technological factor is represented by the type of process and equipment used. From interviews with technical directors over the course of 5 years, they found that non-technological factors—besides small capacities—such as the low priority of implementing energy efficiency measures, prevent improvements in energy efficiency [20].

Missing Data and Information

Furthermore, the lack of information on many opportunities for energy efficiency plays an important role. This barrier is ascribable to the limited time and attention of employees and their limited ability to process information and to make the right decisions [17]. The data basis is often lacking, making it difficult to make decisions on sustainable energy efficiency. Consequently, the collection of data as a basis for decisions is already a challenge [16].

The mentioned barriers are confirmed by numerous further studies and surveys [7, 21–23].

According to Galitsky et al., there are numerous possibilities for the achievement of measures to reduce energy and media consumption [24]. Schröter et al. estimate an energy-saving potential of 15% for manufacturing companies. This corresponds to savings of approximately EUR 5 billion and a reduction in energy consumption of 400 PJ. The most general savings measures are the use of electric motors with speed controls, the recovery of process energy and an intelligent control concept for shutting down systems. Measures such as the use of high-efficiency pumps and combined heat-and-power generation hold further potential for savings. To identify energy-saving potential, it is necessary to analyse the energy weaknesses [7]. A system of indicators for assessing production and energy consumption proves to be useful in this respect. Bunse et al. have worked out a gap between the solutions currently available in the literature and those commonly used in the industry around energy-efficient production processes. The solutions available differ from those implemented at the various corporate levels. To close this gap, IT-supported solutions must be developed to lower the inhibition threshold for investment in energy efficiency [25] and thus to enable companies to make future-oriented decisions.

Since those responsible in production plants should make well-founded and sustainable decisions regarding energy efficiency, a reliable basis for decision-making is indispensable. Decisions should be based on correct data and calculations. The beverage industry is subject to a number of challenges in terms of making decisions. The testing of solutions for energy-efficient work is shied away from due to the necessity of stopping production to do so and due to the risks around process and quality. Innovations for energy efficiency in the beverage industry can be very complex. To be able to apply energy-saving methods and efficiency measures, it makes sense to determine and quantify the respective main consumers of energy and media in the beverage industry. The composition of the complex production process of a brewery will be briefly explained. This understanding is necessary because the numerous chemical and physical interrelationships in the beer-production processes result in restrictions to energy-efficient operation. Also, the following section explains what "energy efficiency" means and what key figures can be used to determine it.

Energy and Media Consumption in the Beverage Industry

Brewing Process and Main Consumers

As mentioned above, the brewing process is an good example of a complex production process in the beverage industry. Due to recognised potential energy savings in the brewing industry, a rough overview of the brewing process and the main consumers within a production plant are required.

The typical brewing process, as shown in Fig. 1, begins with the milling of the malt in the malt mill. The malt grains are mechanically crushed and mixed with water in the mash tun. After mashing in, the mash is heated by several temperature steps. The next process step is lautering, which is the separation of spent grains and wort. The produced wort is heated in the wort kettle and boiled for approximately 1 h [26]. The finished wort is casted out and cooled down via the wort cooler. After completion of the brewhouse work, the cooled wort is pumped into a fermentation tank and mixed with yeast. The yeast starts an alcoholic fermentation and breaks down the fermentable sugars into ethanol and CO_2. After fermentation, the young beer gets matured by storing it at low temperatures to stabilise the beer and reduce off-flavours as much as possible. Before the beer is filled in various containers, most beer types are filtered or centrifuged. The finished beer is put into a bottling tank to store before filling [27].

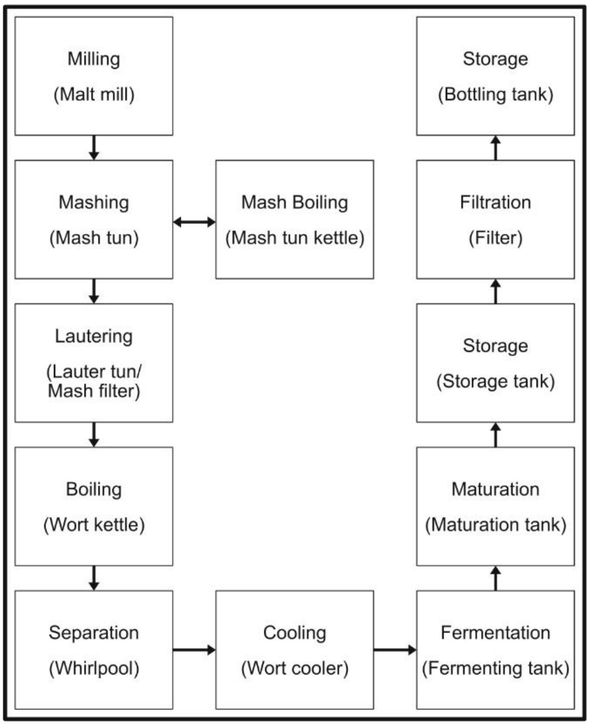


Fig. 1 Brewing process with process steps and typical units

As the brewing and packaging process is a complex and multi-layered process with many heating and cooling processes, various types of energy are required throughout the entire process. The most important energy and media flow in the beverage industry are therefore those of electrical and thermal energy, as well as of water and carbon dioxide. There are only a few sources to be found in the scientific literature concerning precise holistic energy and media consumption data for breweries. The company comparison performed by Schu et al. is achieved by an annual recording of consumption data and enables a comparison of electricity, water and heat requirements [28]. The Dutch brewers' association is pursuing a further approach with a benchmark for breweries with more than

500,000 hectolitres output of beer per year [29]. By using this data and additional environmental reports from numerous German breweries, it was possible to generate the following graph, showing an approximate breakdown of consumption levels in breweries. These values vary greatly depending on the size, modernity and product portfolio of the manufacturing company [28–31].

In the following, the largest main consumers in terms of the individual areas are presented in Fig. 2, sorted by type of energy. Most of the thermal energy in the brewhouse is required by the mash tun and the wort kettle. The second largest consumer is the packaging process. The main consumers here are the bottle-cleaning machine, the tunnel pasteuriser, the crate-washing machine and the flash pasteuriser [31].

In the brewing industry, electrical energy is mainly required for cooling. Most of the power is needed for the cooling systems to cool the fermentation/storage tanks. The demand for cooling power is primarily divided between the wort cooling in the brewhouse and the cooling down of the tank after fermentation [27]. When using a flash pasteuriser during bottling, a high cooling capacity is also required to cool the beer down. The second largest consumer is the packaging process. As Osterroth et al. have shown, the bottle-cleaning machine, the crate-cleaning machine and the filling machine are of particular interest in the operation of a beverage-filling system [32]. In the brewhouse, electrical energy is required especially in the malt mill for crushing the malt. Pumps and motors expect further consumption for the agitators and raking machine of the mash and lauter tun as well as the wort kettle. Another considerable amount of electrical energy is required for the production of compressed air. Compressed air is the most expensive type of energy in the brewery and is produced using electrically driven compressors [14]. Compressed air is mainly required in the bottling step, for switching valves and moving bottles. The two largest water consumers in the brewery are the brewhouse and the packaging. In the brewhouse,

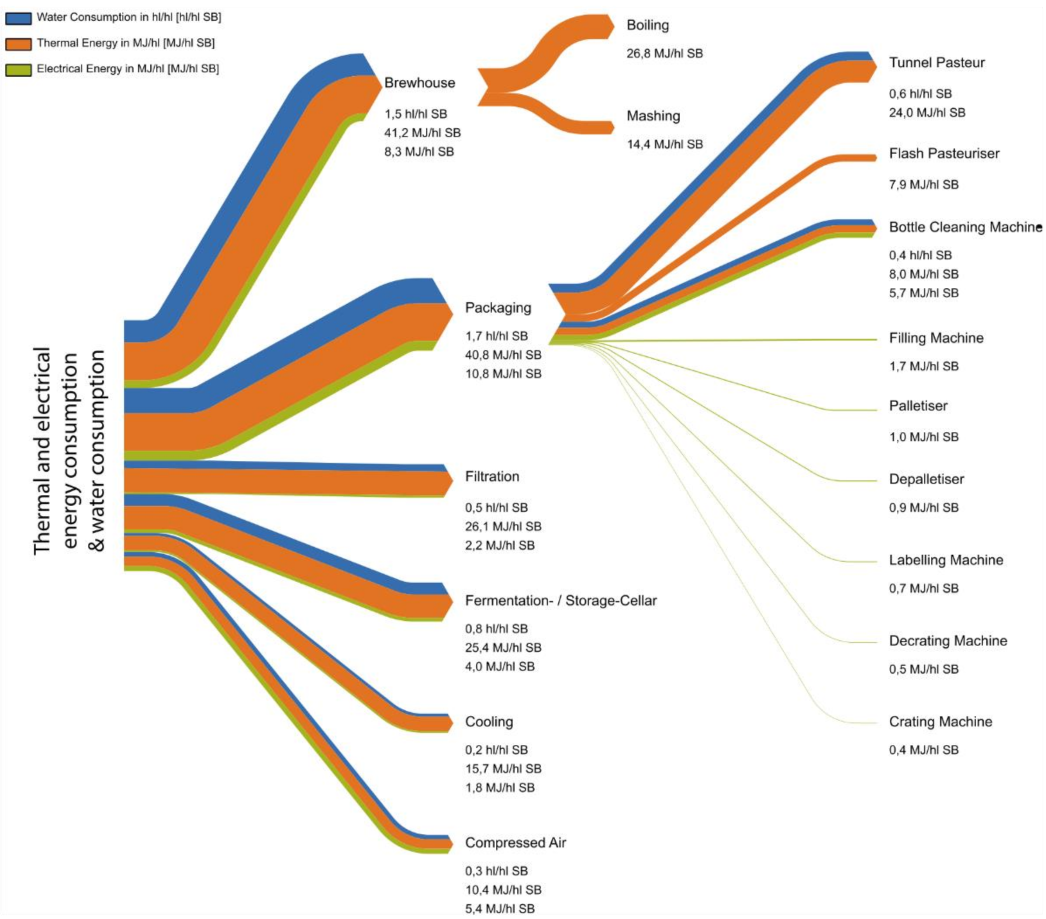


Fig. 2 Thermal and electrical energy demands in MJ/hl (hectolitre) SB (Sales Beer) and water demand in hl/hl SB for process cells and units in breweries (values strongly fluctuating and dependent on plants, processes and products) based on Hackensellner [30], Heuven et al. [29], [32]and Schu and Kern [28] as well as on 22 environmental reports of German breweries

most of the water is needed for the actual beer (mash and sparging water). Only a small part is required as water for rinsing, for spraying the vessels and for emptying the pipes. In bottling, the tunnel pasteuriser as well as the bottle- and crate-cleaning machines are the largest water consumers.

CO_2 is mainly required during filling at the bottling machine and in the area of fermentation/storage and filtration, during pre-tensioning and emptying tanks and the filter. Other CO_2-consuming processes include the filling of a tank truck and the actual serving of beer [27].

Key Performance Indicators for Energy Efficiency

When discussing the energy efficiency of companies, it is necessary to quantify the term. This makes it possible to compare companies, production processes and products in terms of their energy efficiency. This already implies that efficiency can be evaluated on several levels in a production plant by using key performance indicators (KPIs). According to DIN EN ISO 50001 for energy management systems, companies must determine suitable key figures to be able to carry out comparisons. The energy performance indicators (EnPI) mentioned in the standard are a particular form of KPI and are usually represented by specific energy consumption. These EnPIs must be continuously recorded, checked and compared with the starting basis by a Plan-Do-Check-Act (PDCA) cycle [33]. In this way, improved energy efficiency is to be achieved. However, there are no exact specifications as to how an EnPI is to be determined or calculated. Therefore, these indicators are strongly dependent on the respective company.

There are a few approaches in the scientific literature for a generation of custom performance indicators. May et al. propose a seven-step method to develop company-specific KPIs. In the first step, all resources needed for production are defined, and in the next step, their different energy requirements are identified. Thereafter, in the third and fourth steps, the manufacturing states linked with constant or variable values of energy consumption states are determined. On this basis, an energy diagram showing all possible losses and the values which affect a reduction of the energy efficiency was created. The diagram is similar to the classification of time losses while calculating an OEE (overall equipment effectiveness)-KPI for production lines. Based on the chart, KPIs can be derived [34]. Schmidt et al. worked out five different types of KPI, partially based on the work of May et al. They developed a template for each KPI type. The types are, for example, the specific energy consumptions or costs for a unit/product/department, the site energy cost/consumption, the onsite energy efficiency, the improvement or saving of energy cost/consumption/share and finally the total value of energy cost/consumption/contribution. The templates were applied to a case study company, and 14 different KPIs were found. This method enables a statement of energy efficiency to be made at different company levels [35]. Mostly, this analysis fails due to the lack of reliable data [34, 35]. Further, the energy efficiency in industrial processes can be described by the quotient of the output of a process to the energy input to a process as shown in Formula 1 [36].

$$\text{Energy efficiency} = \frac{\text{Benefit}}{\text{Total effort}} = \frac{\text{Product output}}{\text{Energy input}} \qquad (1)$$

Formula 1: Energy efficiency [36].

Measures to Improve Energy Efficiency

Numerous measures can be taken to improve energy efficiency. These can have a direct or indirect impact on energy efficiency. In the following, selected possibilities for improving energy efficiency will be shown. The development of new processes or equipment, e.g. dynamic wort boiling by using an internal boiler [37, 38], has a direct impact on energy savings. Further possibilities lie in energy balancing, process optimisation, heat integration and the integration of renewable energy. A modern brewery can supply its thermal energy demand by using own resources and recuperation [39, 40]. By reducing losses for not only products such as extract and beer, but also materials such as hot water, energy efficiency is indirectly improved, as the quantity of product produced is increased. This also goes hand in hand with the reduction of waste. Furthermore, the behaviour of the employees plays a major role in energy efficiency. Employees should be made more aware, for example, of the use of water during cleaning or the switching off of lights in rooms that are not needed.

The demand for thermal energy can in particular be reduced by reusing energy already introduced into the process [14]. By using pan vapour condensers to generate energy from vapours arising during cooking, the resultant energy can be used, for example for heating the mash water. The use of heat exchangers for wort cooling or the cooling of hot wastewater can result in the recovery of enormous amounts of energy [41, 42]. It is essential, however, that the energy recovered is also used sensibly in the production process. Waste materials can also be used to generate energy [43]. The combustion of spent grains or the anaerobic fermentation of wastewater and the resulting biogas production and combustion in combined heat and power plants are suitable examples [44–49]. The use of regenerative energies, like photovoltaic and thermal solar systems, makes it possible to reduce primary energy requirements [50]. Thermal solar systems can be used to heat CIP systems or bottle-cleaning machines, for example [51, 52].

In addition to increasing the use of regenerative energy for primary energy use [39, 52–55], it is also possible to further use the energy from by-products and to recuperate unused energy and media. Fundamental technological innovations (implementation of concepts) offer enormous savings potential. Considerable potential for savings exists in the brewhouse in particular [42, 48]. Also, consumption peaks can be reduced through organisational factors such as the adaptation and coordination of production schedules. To be able to assess methods and measures for increasing energy efficiency and reducing the media demand in the brewing industry with the existing complex production processes and, if necessary, apply them, a decision-making basis is indispensable. With the help of computer-aided solutions, i.e. analysis and prediction methods, decision-makers can pursue numerous approaches and make well-founded decisions.

Analysis and Prediction Methods in the Beverage Industry

The literature contains numerous approaches to structure a production process according to its energy efficiency [56, 57]. Chaabanee et al. divide such approaches into strategic and tactical levels during the planning of production plants [58]. This is expanded by one level for operations currently running. Each level contains the potential to save energy [59, 60]. The *energy ratio*, which evaluates the ratio of used and invested energy, serves as a measure here [61]. The strategic level deals with the procurement and distribution of energy and resources for several production sites. Furthermore, the location of a factory and the design of the supply chains are determined [59, 62]. Since these strategic decisions are the responsibility of the company and other institutions, and have already been taken during the planning of production, a fixed distribution of the primary energy is specified. Therefore, the strategic level is not discussed further in this work.

The tactical level deals with energy distribution within production and the material flow of raw materials and energy carriers. The operational level deals with the sequence of production processes and their possibilities of increasing energy efficiency [60]. This is also supported by Müller et al. [63] who also present an energy-conversion chain. The chain describes, in a first step, the conversion from primary energy sources (e.g. fossil fuel) to secondary energy sources, which are produced by an energy provider. Further applied energy sources are manufactured by the production company and used to make their products. This means that it is only at the last step, the production system, that optimisation potential is possible for companies, which can also have a positive effect on the first steps. For instance, through an intelligent distribution of the processes that cause peak loads, savings can be achieved in the first transformation steps [56]. This review deals with models for uncovering potential savings and with improvement in the use of energy at the tactical and operational level. Therefore, the origin and type of primary energy do not play a role. The use of renewable energy currently plays an important role and should be kept in consideration.

Energy-monitoring systems form the basis for uncovering savings potential. Their main role is to develop key functions to detect and implement effective energy-saving measures [64]. In order to be able to apply an optimisation strategy to plant systems, it is necessary to gain knowledge about the energy flow and the requirements of individual components. The monitoring of operating processes and parameter acquisition is, therefore, indispensable [65]. Lee et al. divide the different functions of energy management systems in their work into six main groups, which are shown in Table 1, according to their area of competence.

They summarise the results of 276 publications in the field of energy management systems (EMS) and derive a draft for an energy management system for the smart factory of the future by categorisation. The objectives of the EMS are to save energy by back-collapsing both sensors and human feedback, to maintain and expand the supply of renewable energy through intelligent integrated grid control and a combination of EMS and production management to effectively save energy by reducing production waste [64].

Table 2 shows an overview of the relevant scientific publications on the topic of analysis and prediction methods in the beverage industry, by order of publication date. Firstly, the papers are assigned to the following method categories: pinch analyses, simulation, benchmarking, mathematical as well as reference networks and others. Some of the publications cannot be assigned exclusively to one category and are marked accordingly. Secondly, it is indicated which energy and media consumption the publication deals with. The focus is solely on the types of energy and media required in the production process. Also, the process cells in which the respective methods are used in the papers are listed. The hierarchical model structure is defined by the ANSI/ISA-88 [98] and can be further sub-divided. Finally, if specified in the publication, the software or tool used is given.

The following two chapters deal with tactical and operational approaches to energy efficiency in the beverage industry. Based on this, the different methods are critically discussed and compared with regard to the complex problems of different consumers, energy sources, products and media.

Measures on the Tactical Level

Measures on the tactical level aim at the medium-term optimisation of the production process. Simulation methods are mainly used for this purpose. A basis for the implementation of simulation studies is described by VDI-Norm 3633 [99]. The application of simulation studies can have numerous objectives. In addition to the planning of systems and processes, simulations can also be used to answer questions regarding the optimisation of performance and consumption of production

Table 1 Classification of energy-monitoring systems into functional groups at tactical and operational levels, according to Lee and Cheng [64]

	Tactical level	Operational level
Basis function	Monitoring of energy consumption, energy efficiency	
Control function	Demand control	Scheduling, comfort monitoring of human-conducted production steps
Analysis function	Prediction of energy demand	Optimisation, error diagnostics, maintenance control
Management function	Production behaviour	Knowledge management, database administration
Enhanced function	Model-based monitoring	Expert systems, artificial intelligence
Specific function	Process-related	Plant-related

plants during implementation and, above all, during subsequent operation. Figure 3 gives an overview of simulation methods. Deterministic simulation has exact dependencies, whereas random events characterise stochastic simulation. The static simulation takes place at a certain time, while the dynamic simulation is time-dependent. Dynamic simulation can be sub-divided in continuous (continuous change of the system status, using differential equations), discrete (change of the system status at discrete times) and hybrid simulations (mixed discrete and continuous) [100].

In addition, numerous approaches to modelling and subsequent simulation based on reference nets can be found. Furthermore, mathematical modelling approaches used in the beverage industry could be assigned to the tactical level.

Simulation

Concerning the simulation of energy and media consumption, event-discrete and time-discrete simulations can usually be used. Therefore, this simulation technique and scientific publications in the beverage industry will be discussed in more detail in the following section.

On the one hand, in discrete event simulation, each event (change of state) is recorded and reflects the simulation progress. Figure 4 (a) shows an example of this change of state over time. During a change of state, the new state is calculated, future events are planned and, if necessary, a statistical evaluation is carried out. A stochastic behaviour is usually stored for the subsequent state to achieve all possible sequences with several simulation attempts. This is also necessary because the events influence each other [101]. There are multiple attempts in the literature dealing with the simulation of process cells (and especially the packaging process) in the brewery, but not including an energy-based approach [102–106]. On the other hand, in a time-discrete simulation (Fig. 4b), status changes are determined after equal time intervals Δt have elapsed. In the process, status changes between the individual measuring points are not detected. If a small Δt is selected, the state is often recalculated, even if it remains unchanged [101]. In addition, numerous other simulation methods, such as numerical simulation, are used in the beverage industry.

The brewing process can be divided into two sub-areas. The production in the brewhouse, fermenting cellar and storage cellar follows a batch-oriented operating mode, whereas in the packaging area, discrete piecewise production takes place.

Mignon et al. were the first to describe the use of a discrete simulation in the batch area of a brewery. Based on the work by Joglekar and Reklaitis [107], they used the simulation software BATCHES for the batch and semi-continuous processes. Among other things, they examined the influence of the production plan on the thermal energy consumption profile. Based on occupancy times of the individual aggregates and the running production process, it was possible to check two plant modifications and to achieve a theoretical reduction in the number of aggregates. The energy simulation was carried out with the aim of reducing peak loads in the demand for thermal energy, while simultaneously running energy-intensive processes. By changing the period between individual brews, a difference of 46% was achieved between the worst and the best case, in terms of the energy requirement [66]. Based on this work, a Belgian brewery applied the method, in addition to an analytical approach. The goal was to reduce the steam consumptions peaks. By implementing a better standardisation of the equipment in this brewery, choosing an optimal production schedule and limiting steam availability, a 55% saving was achieved, when comparing the best and worst cases [68]. A numerical simulation at unit level for a tunnel pasteurisation machine was performed by Dilay et al. [71]. This is based on a mathematical model (differential equations) including thermodynamic and heat transfer parameters as well as energetic correlations. An optimisation with regard to a minimum energy consumption related to the geometry of the tunnel pasteurisation machine was carried out. The validated results showed savings of 50% electric and 10% thermal energy. In addition to a pinch analysis (see "Pinch analysis"), Müller et al. describe the use of simulation for optimisation in the brewhouse area. They create and simulate an individual model using Matlab&Simulink and the CARNOT toolbox. The simulation experiments investigate the influence of the individual and combined heat sources on the thermal energy-intensive processes in the brewhouse. The energetic

Table 2 Overview of scientific literature references on analysis and prediction methods in the beverage industry

Source	Methods						Energy and media consumption			Process cell				Tools/software
	Pinch	Simulation	Benchmark	Mathematical	Reference nets	Other	Thermal	Electrical	Water	Brewhouse	Cellar/ filtration	Packaging	Utilities	
Mignon and Hermia [66]										x				BATCHES
Ito et al. [67]		x		MILP		Real-Time							x	N/A
Mignon and Hermia [68]										x				BATCHES
Zhelev [69]; Zhelev and Zheleva [70]	x	x							x				x	N/A
Dilay et al. [71]				x				x				x		Prog. with FORTRAN
Waheed et al. [72]						E&EA		x		(x)	x	x		N/A
Johansson et al. [73]								x		(x)	x	x		N/A
Lees et al. [74]		x				RT-UMS	(x)	(x)					x	Gensym G2
Lees et al. [75]						RT-UCM		x					x	Gensym G2
Gahbauer et al. [								x		x	x	x	x	N/A
Dumbliauskaite et al. [76]	x							x		x	x		x	N/A
Fadare et al. [77						&EA		x		x	x	x		N/A
Tokos et al. [78]				MILP		E		x		x			x	GAMS/Cplex
Marty et al. [79										x		x	x	EINSTEIN
Muster-Slawitsch et al. 53 [39]	x x	(x)								x	x	x		T*Sol Expert 4.5
Nagel [80]	x	(x)			x					x				Renew
Bai et al. [81]				x				x	x	x	x		x	Matlab
Sturm et al. [ ]		x						x		x	x		x	ECLIPSE
James and Kariuki [82								x		x	x	x	x	N/A
Yang et al. [83]		x	x					x	x	x	x	x	x	N/A
Forster [84]		x						x				x		N/A
Sturm et al. [ ]			x				x	x	x	x	x	x	x	N/A
Muster-Slawitsch et al. [86]	x						x			x		x	x	SOCO
Muster-Slawitsch et al. [87]				x			x	x		x	x			EES
Marchini et al. [88									x		(x)	(x)		MS Excel/Visual Basic
Hubert et al. [89]		x (x)			x				x	x	x	x	x	N/A
Hubert et al. [90]		(x)			x				x			x		Renew
Pettigrew et al. [		(x)			x		x	x	x				x	Renew
Zogla et al. [92]			x				x			x	x	x	x	N/A
Müller [93]	x	x	x				x	x		x	x	x	x	Matlaband Simulink; CARNOT Toolbox
Hubert et al. [94]		(x)			x		x			x	x			Renew
Hubert et al. [95]		(x)			x		x		x	x	x	x		Renew
Kubule et al. [20]			x				x	x		x	x	x	x	N/A
Kubule et al. [96]			x				x	x	x	x	x	x	x	N/A
Tibasiima and Okullo [97]	x						x			x	x		x	HINT
Osterroth et al. [31]		x						x				x		Matlab and Simulink
Schneid et al. [40]		x					x	x		x	x	x	x	N/A

E&EA energy and exergy analyses, *RT-UMS* real-time utility management system, *RT-UCM* real-time utility consumption model, *MILP* mixed integer linear programming

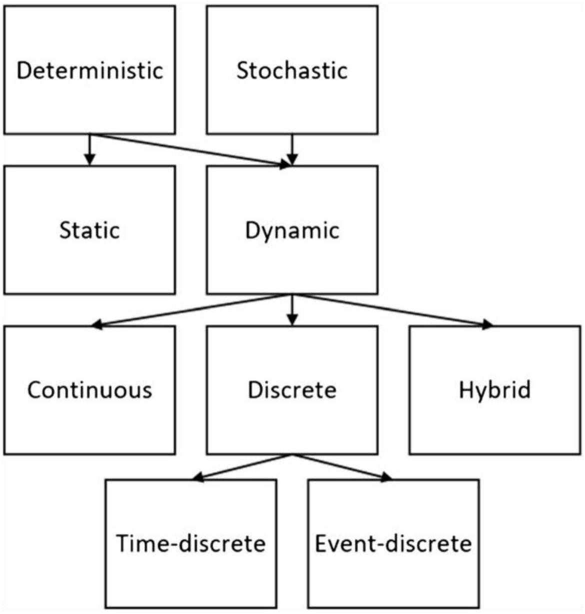
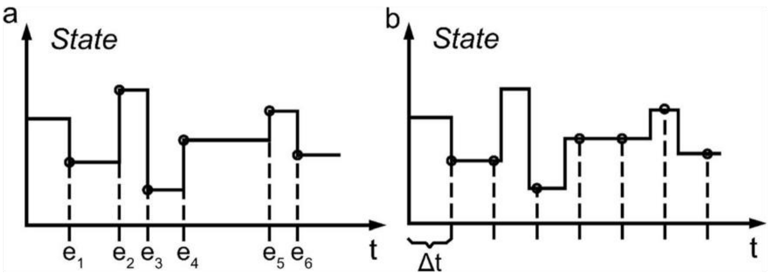


Fig. 3 Overview of simulation methods

optimisation and integration of solar process heat play an important role [93]. Regarding the size of a production plant, Marchini et al. apply a discrete simulation based on Microsoft Excel and Visual Basic in a dairy factory. This example is suitable, as the complexity of the processes in a dairy is similar to those in a brewery. By analysis of the water streams (input, output) and the units, a simulation model was created. Simulation results showed that the implementation of a new tank would generate a water saving of 7.2% [88]. A model for a juice-production system based on DES/LCA and Microsoft Excel is developed by Johansson et al. [73]. The complex production system was modelled around energy consumption, waste and pollutants using numerous parameters and LCA (life cycle analysis) data for each production step. The model was validated by a reference scenario, and the differences discussed. Based on this study, Heilala et al. [108] suggest the combination with the SIMTER tool to provide an interface for all parameters directly in the simulation tool. Concerning the packaging area of a brewery, there are some further publications. Forster et al. broadly describe a simulation approach for a packaging line with regard to electrical and thermal energy requirements as well as the required media, such as water and compressed air. As part of a final thesis, validation was carried out with regard to the electrical energy and compressed air. Unfortunately, there is no further information about the consumption behaviour and the simulation environment itself [84]. Osterroth et al. developed a simulation model, based on the approach that the electrical energy consumption correlates with the operational states of the machines in Matlab Stateflow. The electric energy consumption of a returnable glass packaging line was simulated. They used operational state data from historical data and energetic parameters for every machine as input variables. By defining different consumption (demand) levels for the states of the packaging machines, it was possible to perform a summation of the time per consumption level. The results showed an appropriate fit, using the Theil's inequality coefficient (TIC), for most of the machines: it deviated by only 3–4% from the actual measured value [31]. The summarised contributions deal exclusively with just one part of the brewery and do not represent it holistically. The representation of the entire production site enables a holistic approach. Possible consumption peaks, composed of simultaneously running processes in different process cells of the brewery, would therefore not be visible. Also, all sub-areas of the brewery can be included in the multiple uses of energy and media. Following real-life research, Schneid et al. present the concept of a power-producing brewery. The concept describes an energy-self-sufficient brewery that even generates an excess of energy. To test this concept, a brewery (2.6 mil. hl, all process cells) was simulated throughout 10 weeks, with regard to its demand for thermal and electrical energy. By way of comparison, a model of this brewery with various energy-saving systems and machines was created. In combination with adapted production plans, it was possible to achieve an enormously significant energy saving (especially primary energy). Thermal and electrical load peaks could be significantly reduced or avoided. The implementation of energy-saving measures includes not only the adaptation of production plans but also the recycling of spent grains, e.g. in a biogas

Fig. 4 Simplified graph showing time steps and state changes in event-discrete (a) and time-discrete simulations (b) according to [101]



plant, as well as the use of new technologies such as the hot filling of beer. However, the authors see a barrier to the implementation of such a concept, as the operating time required to supply the biogas plant is 7 days a week. In contrast to other branches of the food industry, this operating time is unusual in most breweries [40].

Reference Nets

In the field of scientific brewing and beverage technology, further simulation approaches to energy and media requirements are available. A further method is the modelling and simulation of plants using reference nets. Reference nets are a further development of high-level Petri nets. Petri nets are models for the description and analysis of processes and systems and are characterised by their simple description, clarity and uniqueness. Reference nets have instances and references within these formalisms. Also, tokens may represent any objects. Using the programming language Java, which can be implemented in reference nets, external classes and objects can be integrated, as can simulations [90, 109]. Corresponding software tools such as Renew [110] make this possible.

There are few researchers working in the field concerning reference nets and simulation in the brewing industry. By the development of a hybrid simulation environment based on reference Petri nets using open source software, Nagel et al. were able to simulate a medium-sized brewery, so as to reduce the steam needs. A modular and straightforward modelling concept enables the representation of a virtual factory. Optimisation, through the operation of the steam boiler, results in an increase in efficiency of 3.8% [80]. Hubert et al. present a reference net–based approach to simulate an optimal wastewater flow in the brewery, in order to reduce the demand for water. Therefore, four different brews and filling processes were modelled. Optimisation of the production schedule was performed using genetic algorithms. Due to the adjusted production schedule, an improvement of 10% in wastewater flows compared to the mean value of all simulation experiments could be achieved [89]. Based on the same method, Pettigrew et al. [91] simulated the water consumption and potential for energy generation from wastewater in a cleaning-in-place (CIP) plant in a brewery. Two different simulation approaches take place: one similar to the real production process and the other with a fuzzy-logic control for the reuse of water. In it, the change in water quality is monitored, and the process water can be separated. The single process steps (within a cleaning process) of the CIP are simulated in detail. Hubert et al. also turn their attention to water demand and wastewater quality in their simulation of beverage-filling plants. Using reference nets, a beverage-filling plant of a medium-sized brewery was modelled and simulated. The model comprises two levels. The first level contains three different scenarios for the lower second level. There, different parts of the bottling line (machines) and their operating behaviour (states) form a simplified model. A comparison of the results against real data takes place and shows similar values and behaviour [90]. In another application of reference nets, Hubert et al. simulate the cooling requirements in a small to medium-sized brewery over the course of 10 months. The wort cooling, as well as the cooling during fermentation and storage of the beer, were considered. The long observation period thus also takes into account other system influences, such as those resulting from raw materials and various recipes. The stochastic model is based on a y-distribution of the total wort quantity, the temperature on a triangular distribution and a Weibull distribution of the total process time in the brewhouse. With regard to fermentation, 130 processes were recorded and a Gumbel distribution determined with the help of the Kolmogorov-Smirnov test. Due to the object-oriented design and the covering of various additional influences, the model is well-suited to the consideration of heat losses in the brewery and to the design of cooling systems [94]. Finally, a holistic approach over an entire production process is presented. Based on the method mentioned above, the modelling and simulation of a unit in the brewhouse are described. In addition to numerous variables, such as volume, temperature and the chemical oxygen demand, the electrical energy demand is also simulated [95].

Further Mathematical Modelling Approaches

Another solution for analysis and prediction methods is the mathematical programming models. These enable the modelling and simulation of versatile and complex application cases, which is why they are suitable for the analysis and prediction of energy and media consumption in the brewing production process. Software is used for this, due to complex arithmetic operations, mixed integer linear problems (MILP) and the solution of differential equations. Numerical simulation is often used for these differential equation–based continuous models. In the following paragraph, tactical approaches based on, among other things, differential equations and energy and exergy analyses are presented.

By using calculations, and energy and exergy consumption patterns, Fadare et al. showed the levels of consumption of electrical and thermal energy in producing a malt drink. With regard to the single production steps, it was possible to work out the main consumers. The exergy analysis showed opportunities for the minimisation of exergy losses and revealed inefficiencies. By far, the biggest consumer with the highest optimisation potential was the pasteurisation process, with 50% inefficiency of the overall system. By increasing the capacity of the pasteur, exergy losses could be reduced [77]. The same results and findings are achieved by Waheed et al.

using energy and exergy analyses for a fruit juice processing plant [72].

Based on the work by [111], Tokos et al. proposed a mixed integer linear programming (MILP) model for heat integration and the installation of a polygeneration system. Similar to a pinch analysis, the model was used to calculate the use of the waste heat. As a result of the calculation, the waste heat from the wort boiling could be used for the heating of the adjunct mash. Furthermore, the heat generated via the clarification of the wort in the whirlpool could be used in the mash tun for heating processes. It took into account the production sequence in the brewhouse to ensure the time availability of the energy. A second simplified model concerns the implementation of a polygeneration plant as described by [112]—ten systems with different characteristics and parameters such as the conversion factor for electricity production. The optimal solution for this use case is a polygeneration system with a back-pressure steam turbine, which produces 50% more thermal energy and covers 42% of the electrical demand [78]. In another model to predict the energy and media demand of a brewery, Bai et al. [81] present a modelling approach of energy consumption using radial basis function networks (as first described by [113]). Combined with a principal component analysis (PCA), a simulation model was created for electrical and thermal energy and for the demand for water and compressed air in the brewhouse and fermentation cellar. There is no concrete example of implementation given. Sturm et al. use CHP (cogeneration heat power) in a microbrewery to investigate energy-saving potentials through spent-grain fermentation and the more efficient use of the biogas in the system through new components (chiller, diesel generator, steam generator). By mathematically and chemically describing the combustion processes of fuels and simulating the material flow through ECLIPSE (a continuous simulation tool), they were able to find out that a newly integrated CHP system, especially in combination with a modern absorption cooling system, has the shortest payback time of the four investigated cases [55]. Muster-Slawitsch et al. [86] present a brewery model on Engineering Equation Solver (EES). A model of the thermal energy demand during mashing, boiling and wort cooling, as well as a model for the cooling demand, was created. The models showed a good correlation, as there are enormous consumption peaks in the thermal energy demand when processes like mashing, pre-wort heating and boiling overlap. By adjusting various brewing process parameters, they tried to reduce the energy demand also to reduce consumption peaks. This would, for example, require a lower capacity for a new design of supply facilities such as the steam boiler. The beers produced with energy-optimising parameters were analytically investigated, but a sensory evaluation is still pending.

Measures on the Operational Level

The operational optimisation of production processes can generally be described by their scheduling. Energy-efficient scheduling can be used to optimise energy consumptions at the production level. There are three main groups of energy flows in the system: energy coverage, energy supply and energy demand [56]. Based on this subdivision, energy-saving potential can be uncovered and efficient energy use made possible with the help of various approaches. Typically, this methodology is based on a variety of components, such as cost and factual factors. With the help of appropriate tools, which are mentioned in the application in the scientific literature in the following paragraphs, established mathematical/stochastic models and algorithms can be solved. To increase the energy efficiency of overall systems, energy recovery is often focused on. Pinch analysis is suitable for this. Also, a comparison using benchmarks and the use of real-time management systems can be used for optimisation at the operational level. These methods are characterised by control and analysis functions.

Pinch Analysis

Operational analysis of production systems can be done using pinch analysis. This method was introduced by Linnhoff et al. from 1979 [114, 115]. A systematic overall picture of all energy flows can be formed based on thermodynamic principles. This paves the way to increasing the thermal efficiency of a production system. With the help of the pinch analysis, optimal solutions can be found through different objectives, such as not only energy efficiency but also economic efficiency and the investment amount. This method is used in numerous fields. In addition to designing new plants or the conversion of plants, existing plants and their operation can also be optimised. In the beverage industry, pinch is used to analyse not only heat exchanger networks, in particular, but also supply systems.

In a pinch analysis, all hot and cold streams are combined with a hot and cold profile and pictured in a temperature/enthalpy diagram (Fig. 5, left). The resulting composite curves are moved so that they are as close as possible to each other. This point is named the pinch and corresponds to the smallest possible temperature difference (ΔT_{min}) for a heat transfer. The temperature difference is justified due to the process and the resulting thermodynamic losses. The exceedances of the curves determine the minimum heating and cooling requirements. The grand composite curve (Fig. 5, right) can be displayed by separating the composite curves, showing where heat is to be transferred and where the process can cover its

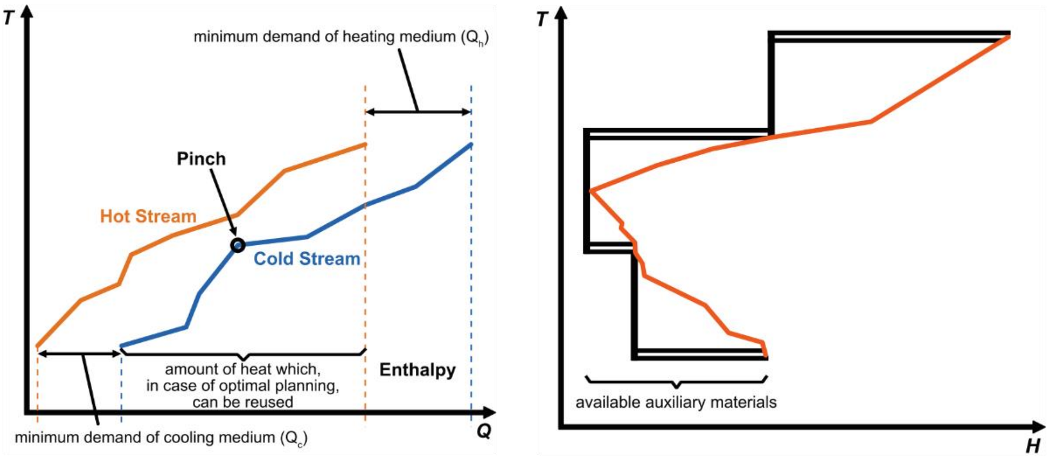


Fig. 5 Exemplary heat balance in a pinch (left) and grand composite curve (right) according to [116]

heat requirements. The temperature differences can be used for transformation processes to reduce the losses caused by the system [116–118].

As these calculations are very complex, especially for complex systems, software tools are used (see PinCH [119], Super Target, Aspen Plus, EINSTEIN ([120]), Hint [121], SOCO [86], etc.). There are numerous articles in the literature that use pinch analysis to optimise processes in breweries.

Dumbliauskaite et al. presented an approach using pinch analysis and revealed a high heat-recovery potential in a brewery by improving the heat exchanger network (HEN). Further calculations concerning economic and environmental factors were performed to determine the optimal setup of the utilities and the integration of CHP and heat pumps. Also, the use of biogas in a CHP system was examined. A reduction of 36% in the costs of heat energy and 44% in CO_2 emission was achieved [76].

Muster-Slawitsch et al. present a concept for a green brewery, whereby they did a pinch analysis for three different breweries as a case study. For one brewery, a detailed pinch analysis was undertaken, concerning all areas of the brewery (hot area, cooling and packaging). Based on the results, a HEN was developed. Concluding, they suggest the importance of heat integration and the use of waste heat. An "energy swing" is needed and is later achieved by [122]. Based on these findings, Muster-Slawitsch et al. developed a pinch analysis tool called "SOCO." They applied a systematic optimisation of the energy consumption of the relevant processes. A simulation of the combined heat integration via heat exchangers and storage tanks in breweries was carried out. The application of the tool on two example breweries showed that 93% of the thermal energy required for the mash tun could be covered by a new HEN system. The residual heat can be used by the bottle-cleaning machine or the tunnel pasteuriser [87]. There are numerous other applications for pinch analysis in different branches of industry [123, 124].

Marty et al. describe the application of the Einstein Audit (as described by [61, 125]) in a large brewery in Switzerland. The brewhouse and the heat transfer network were modelled, and the thermal energy flows mapped. The pinch analysis revealed eight possible new heat exchangers in a HEN. However, the investment costs are disproportionate to the cost savings [79]. Since all calculations are based on the recorded parameters, from which a consumption behaviour is simulated, these are to be regarded partially as critical, since no validation of the data takes place. An industry-specific concept for the green brewery was presented by Gahbauer et al. This is divided into three areas: the preparation of an energy balance and derivation of optimisation measures, process optimisation and a catalogue of measures (BAT—best available techniques) for energy supply. When drawing up the energy balance, benchmarks can be used to identify the need for measures in certain areas. The pinch analysis shows that energy swings must be implemented sensibly. They conclude that heat from the vapour condensate or the heaters of the refrigerating machines should be used instead of hot brewing water, in order to heat the mash water. Thus, the hot brewing water can be used in the packaging area. These findings stand in contrast to Muster-Slawitsch et al. The application of the concept in three Austrian breweries shows, in any case, considerable savings potentials, some of which have already been implemented [53]. Another research on the scheduling of production processes is done by Müller et al. Using pinch analysis, they determinate the optimal schedule for direct heat exchange. Because of multiple restrictions in the brewery, a rescheduling of the processes in the hot area is not feasible. Optimisation potential can be found in the use of indirect heat exchange, which means the implementation of heat accumulators and the decoupling of waste heat from heat demand. With the combination of solar energy, 30% of the thermal energy required in the form of steam can be saved. [93].

Tibasiima et al. use HINT (Heat Integration Software) to optimise the heat recovery of a brewery. For this purpose, the material flows of all hot and cold processes were recorded. Based on this, a design parameter that specifies the temperature range $T_{\min}$ at the heat exchanger interfaces could be selected. By integrating the data into HINT, values for the thermal properties of the process streams were obtained. This resulted in energy savings of 21.5% [97]. However, this modelling is highly simplistic, as losses such as those occurring during heat transfer are not taken into account. Also, the model type TAM (time average model) means that each process step is considered uniformly, and batchwise operation in the brewhouse is neglected. Zhelev also applies a pinch analysis in a South African brewery. The optimisation of heat recovery is performed, taking into account the cooling tower and water cooler structures as well as the HEN topology [69]. Furthermore, they propose a combined water-oxygen pinch analysis for optimisised wastewater management. Thus, the demand for freshwater was decreased by increasing the effluent concentration in central wastewater treatment [70].

Benchmarking

The comparative analysis of values or processes with a statistically meaningful reference value is a simple operative method to uncover potential for increasing energy efficiency [126]. In the brewing industry, numerous associations and institutions offer the possibility of benchmarking. For this purpose, companies can enter their data, in this case, energy consumption data, mostly in online benchmarking tools and receive feedback on the range of individual values in which their own company or process is to be located. This data is usually also published in reports [28, 29, 127]. In the following, the scientific papers concerning benchmarks are presented.

By using E-P analysis (energy production), Yang et al. compared two extension levels (200,000 hl and 280,000 hl) of a Chinese brewery regarding its electric energy and water consumption. Lack of statistical evaluation meant the difference between specific consumption levels could not be proved. Furthermore, there is no information on the articles produced, which have a strong effect on energy and media consumption, within the two periods [83]. A comparison of thermal and electrical energy consumption data of a small brewery (~ 19,000 hl/a) is performed by Kubule et al. [20]. On the one hand, historical energy consumption data were compared using a benchmark from the scientific literature, and on the other hand, the current consumption levels in the brewery were analysed and compared. The historical consumption data of heat and electrical energy in the brewhouse and filling process over 3 years show significantly higher values than the benchmark. This is explained by the size of the brewery and the lack of awareness of energy efficiency. In the second part of the paper, the current heat losses in the brewhouse and the electricity consumption in the packaging area are recorded and classified by type of packaging. The heat losses in the brewhouse are significantly higher than the values given in the literature, which can be attributed to a lack of energy recovery during wort boiling. The specific energy consumption during filling differs greatly according to the type of packaging, whereby filling PET bottles requires significantly more energy than filling glass bottles. Filling kegs is the most energy-efficient variant in this use case. In a further study, the resource and energy efficiency in small and medium breweries were compared. The specific energy consumption concerning the thermal, electrical energy as well the water and malt consumptions are calculated and compared for four different-sized breweries. The values differ, due to various reasons, e.g. the technological standard and produced articles. Using linear regression analysis on a model based on the specific malt consumptions and the beer produced, they were able to predict the energy consumption [96]. Another use case of analysis methods of a brewery is presented by Sturm et al. [85]. The current energy consumption profile is analysed and compared with a benchmark. It shows a large deviation in the thermal energy consumption. In the paper, various measures to reduce the thermal energy demand are presented and calculated. The efficiency can be improved enormously by improved isolation of the containers, as well as the use of the waste heat from wort boiling and the warmth of the exhaust gases of the boilers. The energy demand could be reduced up to 20% with an ROI of 1.3 years. Zogla et al. presented an approach to evaluate the energy performance in the brewing industry. They used the calculation of a theoretical benchmark regarding the thermal heat consumption in the brewhouse for each process and compared the calculated to the real consumption. The resultant energy efficiency index shows the optimisation potential of the production processes [92]. In another benchmarking study [82], energy-saving opportunities were developed. After the data collection in the brewery and the calculation of specific consumptions, measures were derived, and a possible implementation plan worked out.

Real-Time Operating Systems

Furthermore, an approach concerning the control function of the operational level is the application of real-time operating systems. These soft-computing applications work using real-time data directly from the plant. Based on this, intelligent control, diagnostic and decision-support systems can be used to optimise processes and procedures during production to increase energy efficiency. An overview of the purposes and areas of application is given by Campbell et al. [128]. In the following, two approaches from the scientific literature are presented.

Real-time monitoring systems enable the optimisation of processes and procedures during production. Ito et al. provide a method for monitoring the energy-supply system of a brewery combined with an operational decision system based on MILP. The system fulfils two main tasks: the support of the plant operators regarding the most optimal operation mode and the possibility of reducing the operational costs. This can be achieved by the generation of energy, which is subsequently stored in heat accumulators, at times which provide an economic saving [67]. Lees et al. present the application of a G2-based, real-time intelligent utility management system (UMS) in a brewery. The model is used, in one case, for process sequence monitoring, decision support and event management to detect, support and optimise a CIP plant. Due to the UMS reduction of 57%, lower NaOH consumption was achieved [74]. In another case, the model is connected to the PLCs in the production plant to record the current consumption levels. Since metres are not available for every aggregate, the current energy demand was estimated from the current operating status of the individual units. Based on the results, optimal scheduling of production process can be achieved to avoid peak loads and to save costs [75].

Critical Comparison

Numerous approaches are available for the analysis and prediction of energy and media consumption in the beverage industry. These differ not only in the methodology but also in the relevant areas and aggregates of the brewery and in the energy and media types. However, the difficulty lies in finding models that can be universally applied to systems such as breweries, which are complex not only due to the variety of processes, plant types and production lines but also due to the flexible processing of different raw materials and the variability of process parameters. Generally, as a result, there are at the moment only models available that can be applied to specific applications or process steps within the brewery. While pinch analyses are almost exclusively concerned with the optimisation of heat flows and the recovery of thermal energy in the brewhouse area, simulation approaches, such as time- and event-discrete and reference net–based simulations, are ready for application. The presented tactical approaches are very complex in parts and require expert knowledge. This expert knowledge refers to not only the knowledge required for the execution of the simulations but also the understanding of the process. Only benchmarks allow a simple comparison of energy and media consumption. However, there are only a few options for recording benchmarks, and the data basis is limited. The data for the available benchmarks reflect only a small part of the brewing industry. The comparison almost always takes place at site level (brewery as a whole; according to [98]) and at best at a process-cell level. This allows a rough demarcation as to which area has the most optimisation potential but is not suitable for a detailed demarcation. The application of methods such as the mathematically based optimisation of units permits a detailed examination of the system. This makes sense if the result—but not the exact structural relationships—is of interest. Due to their specificity, these models are difficult to transfer to other operations. Detailed considerations require an enormous number of parameters and data. The availability of real data plays an important role in all approaches.

In most cases, there is no (or insufficient) validation of the results with real data. This is usually due to a missing, uniform, industry-specific measurement concept, which would provide data for comparability. Also, it must be clarified which information can be specified to determine the energy consumption of plants. The investigations by Osterroth et al. [31] prove a correlation of the energy consumption of packaging machines with the current operating state. Within operating conditions, time-dependent consumption levels were also determined. The consumption behaviour of aggregates in the batch range is determined in the scientific literature by a large number of parameters.

Although real-time operating systems provide continuous data from the process, they are also only useful for specific applications in individual plants and to improve their energy efficiency. Therefore, they are not suitable for general widespread application.

There are numerous approaches to the application of simulation in various areas of a brewery. The latest approaches address the simulation of an entire brewery in terms of its energy and media consumption [40]. Nevertheless, difficulties lie in the modelling. The numerous commercially offered modelling and simulation environments require a good knowledge of the respective software. Another challenge for simulation is the amount of data and parameters required to obtain a meaningful result and to perform a validation. In general, the number and accuracy of the required simulation parameters increase depending on the level of detail of the simulation. Standardised machine interfaces in the brewing sector, such as the Weihenstephan standard (WS Brew [129] in the batch sector, WS Pack [130] in the packaging sector), can help here. To be able to supply the interface with data, however, appropriate measurement technology is also required, which in turn is associated with costs. Since the willingness to invest and the understanding of energy efficiency are low, especially in small- and medium-sized companies, it is of interest that corresponding software tools with little or no prior knowledge can be used. This is not always the case with the approaches presented.

Conclusions

The current approaches to the analysis and prediction of energy and media consumption in the beverage industry presented in this review paper are based on a wide variety of methods. The reasons for obstacles to energy- and media-efficient working in production plants prove that there is usually a lack of expertise and willingness to invest. Approaches such as pinch analyses, real-time operating systems and mathematical and reference-nets-based simulations require detailed knowledge and can only be carried out by experts. Therefore, these approaches offer an enormous optimisation potential and have a high level of detail. We are of the opinion that only holistic approaches can remove the obstacles and satisfy the needs of the relevant manufacturing companies. Thus, simulation offers the possibility of investigating complete systems in terms of the consumption of energy and media. For example, the main consumers can be revealed and consumption peaks determined. The simulation makes it possible to forecast energy and media consumption in the event of changed production plans and plant configurations. On this basis, measures or investment decisions can be determined and partly quantified. Since the modelling and simulation of production processes such as the brewing process are very complex, we draw the following conclusions as to what an analysis and prediction approach should include. A flexible and context-free modelling environment should be created, which allows the operator to represent a production plant in a simple and understandable way. Modelling of different basic pillars, such as plant model, process model, recipe model and production plan model, is useful. This allows, for example, new articles or processes to be easily modelled and integrated into an existing overall model. To simplify the operation of a modelling environment, extensive component libraries containing the typical plants and process steps in the brewery would standardise the model creation and make it considerably easier and faster. Since the commercially available simulation environments are usually very complex and require operational know-how, a modelling environment should have an interface to such a simulator in which the simulation model can be automatically generated and simulated. A hybrid simulation enables a holistic approach towards the analysis of the efficiency of production plants in the brewing industry in terms of energy and media consumption. This should lead to an increased use of corresponding methods and further advance energy and media savings in the beverage industry.

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2.2 Publication II – Development of a metamodel and software for a holistic model of production plants

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Simulation is a possibility for the investigation of complex production systems like the brewery regarding their energy and media demand and enables the testing of different optimization measures. The creation of simulation models poses particular challenges, since special know-how is usually required. In addition, a comprehensive data basis is required to determine the simulation parameters, which have not yet been defined.
This paper presents a metamodel as a framework for the representation of holistic and hybrid production systems such as the brewery in a standardized and generic way. The metamodel is described in UML and is based on four modeling pillars (physical-, process-, article/recipe-, and production plan model) comprising the complex structure and the needed simulation parameters. The metamodel is transformed and implemented in a user-friendly modeling tool, which enables a simple hybrid modeling without prequalification of the user and allows the wider use of the method which in turn provides for a larger fact base for further scientific developments. Subsequently, a standardized data exchange file, as basis for a simulation model, is generated. The approach is validated via use-cases in a systematic test and by the application for two simulation studies within the different areas of a brewery. It is proved, that the presented approach provides the opportunity to create a holistic model in terms of forecasting energy and media demand.

Contributions of the doctoral candidate (CRediT):

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A metamodeling approach for the simulation of energy and media demand for the brewing industry

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Abstract

Due to economic, social and technical trends, as well as rising energy costs, the food and beverage industry is challenged to work energy-efficiently. Small and medium-sized enterprises in particular lack of both time and knowledge to identify and implement suitable energy efficiency measures. With the help of simulation, decision-makers can pursue numerous approaches and make well-founded decisions. A metamodel based on four modeling pillars (physical-, process-, article/recipe-, and production plan model) for an entire production system concerning the forecast of energy and media consumption is presented. The metamodel is implemented in a user-friendly modeling tool, which enables a simple hybrid modeling without prequalification of the user. Subsequently, a standardized data exchange file, as basis for a simulation model, is generated. For validation, various use cases were modeled and the tool was validated using a systematic test. In addition, two simulation studies were performed to show that the presented approach provides the opportunity to create a holistic model in terms of forecasting energy and media consumption.

KEYWORDS

brewing industry, energy demand, metamodel, modeling, simulation

1 | INTRODUCTION AND OBJECTIVE

The energy-intensive production of food and beverages is a challenge to the manufacturing industry due to political, economic, environmental, and social conditions.[1,2] The high market dynamics, which require a large product range and extremely flexible production, are special for the beverage industry. Through energy-efficient production, costs can be sustainably reduced and competitiveness can be increased.[3,4] In the last few years, there have been enhanced attempts to further develop beverage production in terms of technological performance or to improve its energy efficiency. This is often achieved using catalogues of IT-based measures and software tools.[5–7] In an earlier work of the authors, various methods for improving and uncovering optimization potential concerning energy and media efficiency in the beverage industry were examined. It was shown that the application of simulation, compared to other methods, proves to be most suitable for a holistic analysis to uncover optimization potentials and to test different scenarios. Its advantage is that complex, cost- and time-intensive real experiments, which result in a stop of production, can be avoided. Especially in connection with a production plan, simulation studies allow the greatest possible flexibility.

Previous approaches are either limited by their focus on only one type of energy and mostly serve only partial areas of production or the underlying model as the basis for validation is not sufficiently realistic or only incomplete.[8] There are numerous challenges in the implementation or application of the software solutions, which mostly lie in the generation of models. These are related to the creation itself, but also to limitations caused by the companies, especially small and medium-sized enterprises (SMEs), themselves. This is reflected in the lack of financial and human resources.[9] Therefore, the precise specialist know-how in the field of modeling and simulation is often missing.[10] Also, the amount of required data and parameters is very important, especially when mapping an entire production plant. An upstream problem is usually the missing information along the process chain and the plants and machines.[11] The beverage industry is characterized by a high complexity due to the number of devices and machines, different production processes, which are dependent on biological and chemical influences, and the high speed of packaging processes. Due to numerous heating and cooling processes, the brewing process is one of the most energy consuming manufacturing process in this industry sector.[1,12] Precise knowledge of its processes is essential to meet the required product quality and optimize the process efficiency.[13] Furthermore, the German brewing industry, for example, is characterized by SMEs (yearly production <50.000 hl), as they represent approx. 90% of the companies.[14]

Based on the results of the authors previous literature work,[8] a modeling approach for uncovering the potential for increasing energy and media efficiency by simulation is proposed. The prerequisite for this is a formal description and definition of a uniform data structure for the system. A metamodel is a suitable approach.[13] It should set the framework to represent production plants holistically in a generic and hybrid way. Consequently, it could be used for all different companies in the beverage industry. Concerning the recording of the parameters required for simulation, such as information about material flow or energy and media consumption, no standardized procedure has been available to date. Furthermore, by describing the required data basis and structure, a metamodel can provide first principles for this. Moreover, a combination of batch-oriented and discrete operation in the beverage industry is not described in a model yet.

This paper presents a holistic, generic and hybrid modeling approach for production systems in the brewing industry with regard to the energy and media consumption. Consequently, a metamodel, covering all production areas, as well as production processes, articles, recipes and the production plan, is presented. This should serve as a basis for the creation of models, which map the structure and all required parameters needed for a later simulation. To achieve this, a software solution, which incorporates the metamodel elements, is presented. The aim of the modeling environment on the one hand is a simple and fast creation of models without specific prior knowledge and expert know-how and on the other hand the possibility of favorable forecasts for energy and media consumption. This can be achieved by the generic model, which should represent any variants of production systems. As a result of the modeling environment, an exchange format containing all relevant simulation parameters is created. This provides the basis for an easy creation of simulation models, independent of the simulation environment. Subsequently, simulation experiments can be performed. The application of the metamodel is shown with examples from production companies. The modeling environment is validated with respect to the requirements, especially with regard to the barriers of SMEs. In order to demonstrate the suitability of the overall methodology exemplary simulation studies for the batch and the discrete area were carried out.

2 | THEORETICAL PRINCIPLES

2.1 | Beer production and packaging process—challenges for modeling a production system

According to the German Purity Law, only the four raw materials, malt, water, hops, and yeast are allowed be used to produce beer. In the following, the beer production and bottling process are briefly outlined, with details about the main systems and processes involved. The production process in the brewhouse begins with the milling of the malt in the malt mill. The next process step is the mixing of the grist with warm brewing water in the mash tun (mashing). The mash is heated in different temperature ranges for a certain time and then lautered in the lauter tun. During this solid–liquid separation, the husks are separated from the wort. The wort produced is heated and cooked in the wort kettle for about 1 h.[15] Afterward, the wort is cast out and cooled down by the wort cooler. The gained heat can be reused in the process, for example, for mashing. Depending on the configuration of the brewhouse, the number of brews per day may vary. The bottleneck of a brew house is the lauter tun. When the brewhouse work is completed, the cold wort is pumped into a fermentation tank and yeast is added. The yeast starts the alcoholic fermentation and decomposes the fermentable sugars into ethanol and CO_2. The CO_2 obtained is processed and can be reused at numerous points in the brewery. During the fermentation process the tank is cooled continuously. After fermentation, the young beer is stored in storage tanks to stabilize and eliminate off-flavors. Most beer types are filtered or centrifuged. The finished beer is then pumped into bright beer tanks and is ready for bottling.[16]

The challenges in modeling the batch area of the brewery lie in the numerous different plant combinations or sizes as well as the different production process possibilities. These vary depending on the requirements for the beer style being produced and on their quality requirements. Some examples are described below: In the brewhouse, for example, a lauter tun or a mash filter based on the principle of pressure filtration, may be used.[17] Besides an infusion mashing process, a decoction mashing process using a mash pan may be utilized. In the second alternative, one part of the mash is boiled up in the mash pan and then returned to the original mash. There are numerous possibilities when choosing the boiling system. Besides the use of a wort kettle, as described above, systems such as thin-film evaporation or a gentle boiling system can be used. The approaches for fermentation and storage of beer vary from single-tank processes in cylindroconical tanks to the use of three tanks for fermentation, maturation, and storage. In the production of beer, many different approaches and possibilities are pursued in terms of plant configuration and process control.[18] These approaches vary greatly depending on the size of the company as well as the variety of products. For example, a microbrewery producing up to 1.000 hl per year has a different number and size of devices than a large brewery producing several million hl per year. The quality of the products also has a decisive influence on the production processes and the choice of equipment.[19] The challenge of modeling the batch area of the brewery lie in the representation of all possible plants and their combinations. Besides this, it must also be possible to adequately model all processes in terms of their energy and media requirements.

The plant structure of the packaging area varies depending on the type of packaging (e.g., kegs, bottles, and cans), the packaging material (glass, PET, and aluminium), and the packaging concept (disposable and reusable).[6] Manger et al.[20] describes the variety of machines in beverage bottling plants. Due to the high complexity, the plant structure of a bottling plant for returnable glass bottles is described below. Buffer conveyors connect the individual machines. In combination with increased output of the central unit, usually the container filling machine, those conveyors serve to buffer any pre- and succeeding failures in order to ensure trouble-free production. The empties in crates brought into the beverage bottling plant must be unstacked from a pallet by the depalletiser. The emptied crates are transported by a crate conveyor to the decrating machine, which has the task of unpacking bottles from the crates and placing them on a container conveyor belt. This conveyor belt transports the bottles to the bottle-cleaning machine, where they are cleaned and disinfected after which they are ready for refilling. The empty crates are also cleaned and transported directly to the crating machine. The cleaned bottles are inspected for various features by the empty bottle inspector after which they can be filled with the appropriate product and sealed in the container filling and sealing machine. Afterward, the bottles are provided with labels by the bottle labeling machine and are repacked into the cleaned crates in the crating machine. These are then stacked on pallets by the palletiser and transported from the plant to the warehouse or logistics. A summary of the main consumers in the individual production areas according to energy and media type is presented by Bär and Voigt.[8] A detailed investigation regarding consumption in the packaging sector is described by Osterroth et al.[6] in a representative survey. Their work provides a good overview of the individual main consumers as well as the consumption structures. The challenge in modeling the packaging area lies in the mapping of different machine types and their different parameterization. These vary above all depending on the container type to be processed and its corresponding further packaging. The different process equipment for preparing the product to be filled and the transport equipment used within the system must also be considered.

2.2 | Dependency of the energy and media consumption of the different production areas

The two production areas differ not only in their different production methods, but also in their dependence on energy and media consumption. In the batch area, the demand for thermal and electrical energy, as well as media such as water, compressed air, and CO_2, depend on the respective process. Consequently, approaches for modeling the batch area of a brewery refer to process modeling.[21–24] As Muster-Slawitsch et al.[25] have shown, the energy is required at certain times in the process. Due to simultaneously running processes and the superposition of consumptions, enormous load peaks can occur.

In the packaging area the energy and media consumption depends on the current operating state of a machine. Based on works on discrete working machines by Cataldo et al.,[26] Osterroth et al.[27] proved that different energy and media consumption levels of packaging machines in the beverage industry relate to the current operating status. They defined corresponding consumption levels, which furthermore show a granular distribution of consumption levels concerning time dependency within a given state. The available operating states and a state model are described by the Weihenstephan Standards, a definition of a data interface for packaging machines.[28]

2.3 | Application of standards for the classification of production plants

The production of beer takes place in a batch-oriented discontinuous way, as described in ANSI/ISA S88.[29] This means that the same batches of beer are produced on specific plants using processes defined by recipes. Discrete manufacturing is used in the filling and packaging area of a production process. Here a piece-by-piece production takes place through the same work steps of the individual machines. The ANSI/ISA S88 describes standards for structuring a production plant by mapping the individual models to hierarchical levels. Figure 1 shows the subdivisions in levels of the physical model on the left side and process model on the right side. The dotted arrows also show the mapping to an example from the brewing process.

The physical model describes the physically existing plants and machines of a production plant. The relevant top-level comprises *process cells*, which consist of several subsystems required for the production of a batch. The second level describes *units*. An example for a unit in a brewery is a vessel such as the mash tun. *Equipment modules* are subordinate. These carry out several small process steps within a unit. The lowest level is described by *control modules*.

The process model is also divided into four levels. The highest hierarchical division is the *process*, which comprises a sequence of steps to produce a single batch. It is subdivided into *process stages*. In these steps, so called *process operations*, which lead to a chemical or physical transformation are summarized. The lowest level is described by *process actions*. Furthermore, a mapping of the process model to the physical model can be derived from the S88 standard (dashed arrows). A process may only run on one process cell. In addition to a process stage, a unit can also be linked to process operations and process actions. Process actions, on the other hand, can also be executed on an equipment module.

Despite the different production methods in the packaging area, the S88 standard can also be applied here. Since the machines always work in the same way, no process model can be defined, but the division of the physical model can be transferred. In this case, a process cell corresponds to an entire packaging line. This means

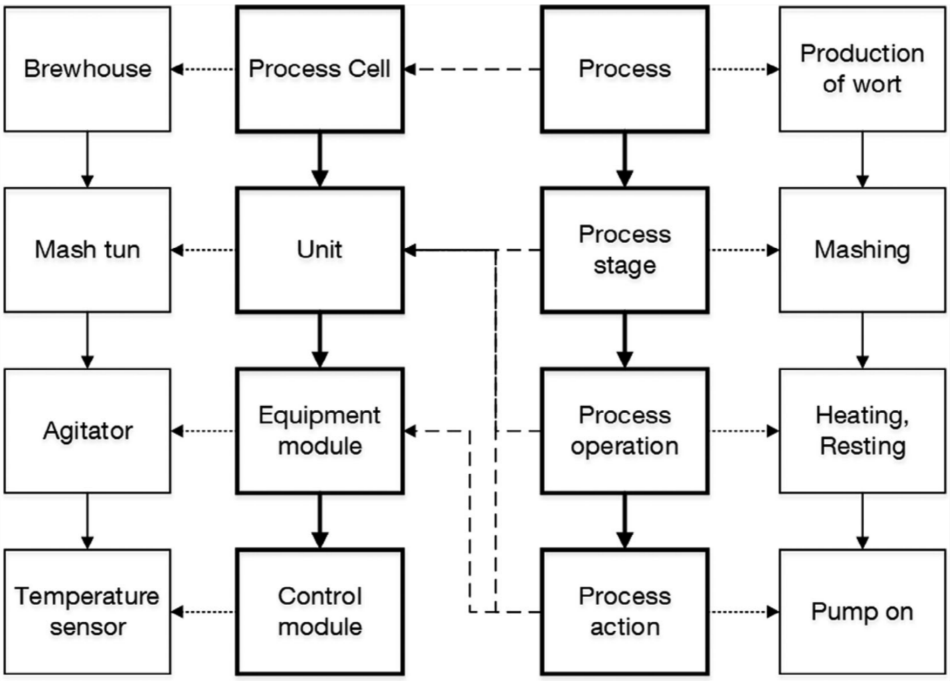


FIGURE 1 Hierarchical subdivision of the physical (left side) and process model (right side) according to ANSI/ISA S88; dashed arrows show the possible mappings of the two levels; dotted arrows show an example of the respective level

that individual machines, such as the container filling machine, can be classified as units. Equipment modules represent individual motors or pumps. Control modules represent sensors.

2.4 | Modeling of production systems for the simulation of the energy and media demand

The VDI 3633 norm defines a guideline for the procedure for simulation studies. The "preparation" development phase therefore also includes data determination and coordination as well as the creation of the simulation model. A model is an abstract representation of a complex problem or system, in which clear system boundaries are defined. The degree of detail is a measure of the accuracy with which a system is depicted in a model.[30] A model thus has the function of depicting or designing complex systems more easily and is the result of a construction process in which the perception of the contents of a selected object is presented in a purpose-oriented way.[31] Important for the simplification of a real system is the previous definition of the purpose of the model. Dangelmaier[32] therefore describes system optimization with regard to system structure, behavior and function.

Metamodels can be used to gain a better understanding and generalization of the system. A metamodel represents only the essentials and serves to simplify the model. As a result, metamodeling is a practical but robust tool for interpreting and analyzing highly complex models.[33] Simulation is usually only used for complex systems, which cannot be represented by mathematical-analytical methods. Since simulation can only be achieved by creating a model, the definition of a metamodel offers numerous advantages.

The scientific literature describes different approaches and methods concerning the modeling for simulation of energy and media consumption of beverage production systems. There are way more simulation and optimization approaches in the food and beverage industry regarding product quality and process optimization, but this will not be the subject of this publication. Supply chain models also provide a differentiated view of production systems, since business, delivery and decision-making processes are usually relevant.[34,35] In the following, relevant publications in terms of energy and media consumption are briefly presented and the necessity and requirements for a metamodel are derived.

For the brewery, numerous approaches using a pinch analysis, an analysis of the thermal energy flows and determination of the energy available for use, are described. Mostly heat-exchangers or the integration of cogeneration plants are the objects of investigation.[5,36,37]] Mignon & Hermia[21] used the software BATCHES for modeling and simulation of a brewhouse. The modeling in this tool is based on plants, recipes and production plans according to ANSI/ISA S88. The influence of the production plan on the thermal energy demand of the units of the brewhouse could be investigated. In addition to the investigation of the optimal plant configuration, an energy simulation was used to reduce the peak thermal energy demand. This method made the reduction of a brewery's primary demand for thermal energy possible.[22] Based on the software Engineering Equation Solver (EES), Muster-Slawitsch et al.[25] modeled plants, processes, energy flows and the production plan of a brewery. Their presented models represent the thermal energy demand during the brewhouse processes and the cooling load of a brewery. In both cases, significant consumption peaks could be detected, which were tried to be minimized by changing the process parameters. Dilay et al.[38] use numerical simulation to optimize a tunnel pasteuriser in beverage filling. By modeling the water and heat network a statement about the energy consumption in connection with the plant geometry could be made. Another possibility for modeling and simulation is via petri nets. Petri nets are models for the description and analysis of processes and systems. They are characterized by their simple description, clarity, and uniqueness. With the help of Java, which can be implemented in reference nets (a further development of high-level petri nets), simulations can also be performed. Using a simulation through reference nets, Nagel[39] was able to reduce the steam requirement of a brewery. The modeling was carried out using a graphical and modular software tool. Hubert et al.[40] carried out modeling based on reference nets concerning the reduction of the water demand of a brewery. The processes taking place were modeled in reference nets and genetic algorithms were used to determine an optimal production plan. Using the same method, Pettigrew et al.[41] simulated water consumption and the potential for energy production by treating wastewater in a brewery. Hubert et al.[42] also modeled and simulated the water consumption and wastewater quality of beverage bottling plants using reference nets. The modeling included the individual aggregates of the beverage bottling plant and their operating behavior in a simplified form. The cooling demand of a medium-sized brewery was simulated over 10 months based on reference nets. The ongoing processes were modeled using a two-level hierarchy. Furthermore, Hubert et al.[43] presented a holistic approach to modeling and simulating a brewery, based on the concept already mentioned. Among other things, the entire electrical requirements of the production plant were simulated.

Modeling and simulation of energy and media consumption is also applied in other industrial sectors using diverse tools. Li et al.[44] deal with the petri net representation of the ceramic production process, which is characterized, similar to the brewing process, by the application of batch-oriented and discrete operation. The production of bio-ethanol with regard to energy efficiency is modeled and simulated using the commercial software Aspen Plus. Therefore, the production processes are depicted and simulations regarding different use-cases are performed.[45] The simulation and optimization of electrical energy consumption of manufacturing processes can be performed using the software Arena, and should serve as a good example for an easy to use tool, especially for SMEs.[46] A discrete simulation based on Microsoft Excel and Visual Basic in a diary factory with regard to the water consumption by modeling all water streams and relevant units is done by Marchini et al.[47] Tokos et al.[23] uses a mathematical integer linear programming (MILP) model to analyze energy saving opportunities in a brewhouse with regard to heat integration. The MILP model was solved using the software GAMS solver Cplex.

Further publications concerning modeling and simulation in the brewing industry deal with the bottling area. Forster[48] describes an approach to simulate a packaging plant in terms of its energy and media consumption. The modeling is based on a specifically developed block library in Plant Simulation, which intends to increase flexibility concerning the level of detail and to provide a large number of machines and transport systems typical for this industry. Osterroth et al.[27] used Matlab-Stateflow to model and simulate the electrical energy consumption of the machines depending on their operating behavior. In this work, a simulation model based on the hypothesis that the electrical energy consumption of machines depends on their operating state and is within time-dependent was developed. By defining consumption levels, a very good concordance with the real data could be achieved.

A few papers deal with a similar approach for depicting a production system and therefore are useful for this work. Weissenberger et al.[49] presented an interesting approach for modeling production plants in the beverage industry, by which a manufacturing execution system (MES) may be automatically generated. This involves, among other things, the modeling of plants and processes. The modeling approaches are based on existing standardizations and thus provide a good basis for this work. Chen et al.[50] describe the application of the method in the brewery and also present a software solution for modeling.

It can be concluded that a wide variety of methods for modeling production systems concerning energy and media consumption or its optimization have been used for the domain of beverage production. All modeling and simulation approaches have in common that they do not cover the entire production system. In the case of the brewery, only sub-areas, that is, batch- or bottling area, were represented. Moreover, none of the approaches consider all energy and media consumptions of a plant. Only Forster[48] describes a holistic simulation in the packaging sector. In the batch area, the most frequent investigations are carried out in the brewhouse regarding the consumption of thermal energy. Especially the mapping of both production areas is a great challenge due to the different production methods and energy and media consumption dependencies. Approaches for structured and generic modeling can only be found in references[49,50] but with a different focus. Approaches to the information and parameters required for a model are described by references,[21,27] in each case area-specific. Currently, no (meta-)model, which includes the required information and parameters, is available for the holistic depiction of a production system of a beverage company. Although numerous tools and special software are used for the modeling, as described above, these are only of limited suitability, since on the one hand both production areas cannot be represented and on the other hand the operation, that is, the model creation requires special know-how and previous knowledge of the operator. Especially for SMEs, this is a barrier.

Consequently, the authors propose a metamodel based approach for the simulation of production systems in the brewing industry with regard to energy and media consumption. The structured and generic metamodel creates a basis for all simulation-relevant information and parameters. To enable an easy model creation and to overcome the barriers of SMEs, a software implementation of the metamodel is presented.

3 | MATERIALS AND METHODS

3.1 | Metamodeling in UML

The metamodel for production plants concerning the simulation of energy and media consumption is depicted using class diagrams in the graphical unified modeling language (UML) and is done with the commercial software Visual Paradigm Version 14.2 from Visual Paradigm International. Usually, UML is used in model driven software engineering approaches for the modeling of software systems but is nevertheless suitable for the representation of data models. The advantages of UML lie in defined terms and relationships and the resulting clear model specification of model components. Class diagrams, in particular, are convenient in the regarded case to represent the metamodel consisting of classes with attributes, interfaces, and relationships.[51] Classes comprise objects that are structurally identical and therefore have the same attributes. This abstraction allows the modeling of a delimited system. A class is represented by a rectangle with the name of the class. All attributes of this class are added to the rectangle. There can be numerous interfaces between classes, which describe the relationships. A general association (single arrow) represents relationships between classes or objects of classes. A composition (arrow with black diamond) means a special aggregation, which describes that parts cannot exist without the whole and are therefore existentially dependent on it.

3.2 | Transformation from UML to XSD

The graphical and formal notation of UML allows representing the complex structure in an XSD (XML Schema Definition). Since the Extensible Markup Language (XML) is recommended as an exchange format, for example, between the modeling environment and a simulation environment, the advantage is that XML files can be described and thus verified by XSD. This also reflects the advantage of XML, which is a format for structuring and exchanging data and can be described in an application-specific manner using XSD.[52] Other advantages of XML are its usability for a platform implementation-independent exchange of data and its good readability by man and machine. Numerous transformation patterns are available for the automatic transformation of UML to an XSD.[53,54] Starting from the metamodel, the transformation to an XSD for the description of the final data structure and the data content of the transfer file was carried out. The XSD has been edited using the commercial software <oXygen/> XML Editor 20.0 of Syncro Soft SRL. The advantage of describing the XML file via a schema is the description of the relationships, constraints and the order of data. In addition, classes or elements can be defined and their attributes, that is, content, data types and the unit, can be specified.

3.3 | Development of a modeling environment

Based on the metamodel presented in UML class diagrams and the XSD for the formal description of the XML exchange file, a software-technical implementation could be performed. The implementation was done by object-oriented programming in C++ in the development environment Qt Version 4.10.2 (an application framework and GUI toolkit) by The Qt Company.

3.4 | Systematic test for validation of the modeling editor

According to Schultewolter,[55] a systematic test was carried out to evaluate the software-technical solution with the mentioned requirements, especially in SME. The validation and assessment in different factors for a modeling editor was performed based on Chen et al.[50] 20 test persons, which covered a representative range of participants, as they had different levels of knowledge and previous experience in the field of modeling, were acquired to independently create and parameterize a model in the editor according to a given task. The tasks included all four modeling pillars as well as the interfaces between the individual models and thus provided a cross-section. As a first step, the test group was asked to model a brewhouse and a beverage bottling plant consisting of several elements as physical models. This includes the creation of a new element as well as the parameterization of the units. In the process model, two processes consisting of several process stages should be created and the process operation should be parameterized. Both processes were then assigned to the units of the modeled brewhouse in the recipe model. Two different articles had to be created in the article model and numerous machines of the beverage bottling plants had to be parameterized with corresponding article-dependent parameters. Finally, a production schedule had to be created for each production area. Additionally, a shift plan and corresponding mashing rhythms, as well as changeover/cleaning times, had to be inserted in a matrix. Following the systematic test, a questionnaire was drawn up. The poll included questions on previous experience with modeling and subjective impressions as well as the comprehensibility of the modeling approach and its implementation in terms of user-friendliness. The suitability of the modeling approach and the editor should be determined on the basis of the following four factors, see Table 1. The evaluation of the individual criteria should allow conclusions to be drawn about the usability and further benefits of the modeling tool.

4 | RESULTS

4.1 | Generic metamodel for production systems with regard to energy and media consumption

Figure 2 shows an overview of the individual sub-models of the metamodel, presented in separate columns. The illustration in individual independent columns allows the hybrid and context-free modeling. The model columns correspond to the categorization according to ANSI/ISA S88.[29] The modeling approach refers to the unit level in the physical model and the process operation level in the process model. A more detailed approach might present the simulation of the overall system in more detail but would require an enormous increase in data and parameters. As a result, it would be too complex for the presented holistic modeling of complete production plants. The linking of the models with each other allows the representation of different recipes and articles with varying energy and media consumption. This flexibility allows the most realistic representation possible, which is necessary for the exact simulation of an entire production system.

The first column describes the physical model. Within this metamodel, a distinction between the model for batch-oriented operation and discrete production can be made. Units are represented by different classes, which also differ in their energy consumption behavior. The process model describes the running processes in detail down to the process operation level. The recipe model comprises, on the one hand, the recipes, which assigns processes to the respective process cells and units of the physical model. On the other hand, all articles, which can be produced on the discrete working plants of the physical model, are included. The fourth pillar, the production plan model, describes the production sequence, that is, the sequence of different recipes and articles on

TABLE 1 Validation criteria for the modeling editor (following Chen et al.[50])

Criteria	Evaluation contents
Simplicity	Simple and fast creation of the models
Comprehensibility	Modeling approaches and models are comprehensible and understandable Model creation without specific knowledge
Completeness	Modeling approach covers the requirements and scope of the individual modeling areas
Sustainability	Extent to which the modeling approach can be used (e.g., in other industries due to modification and extension)

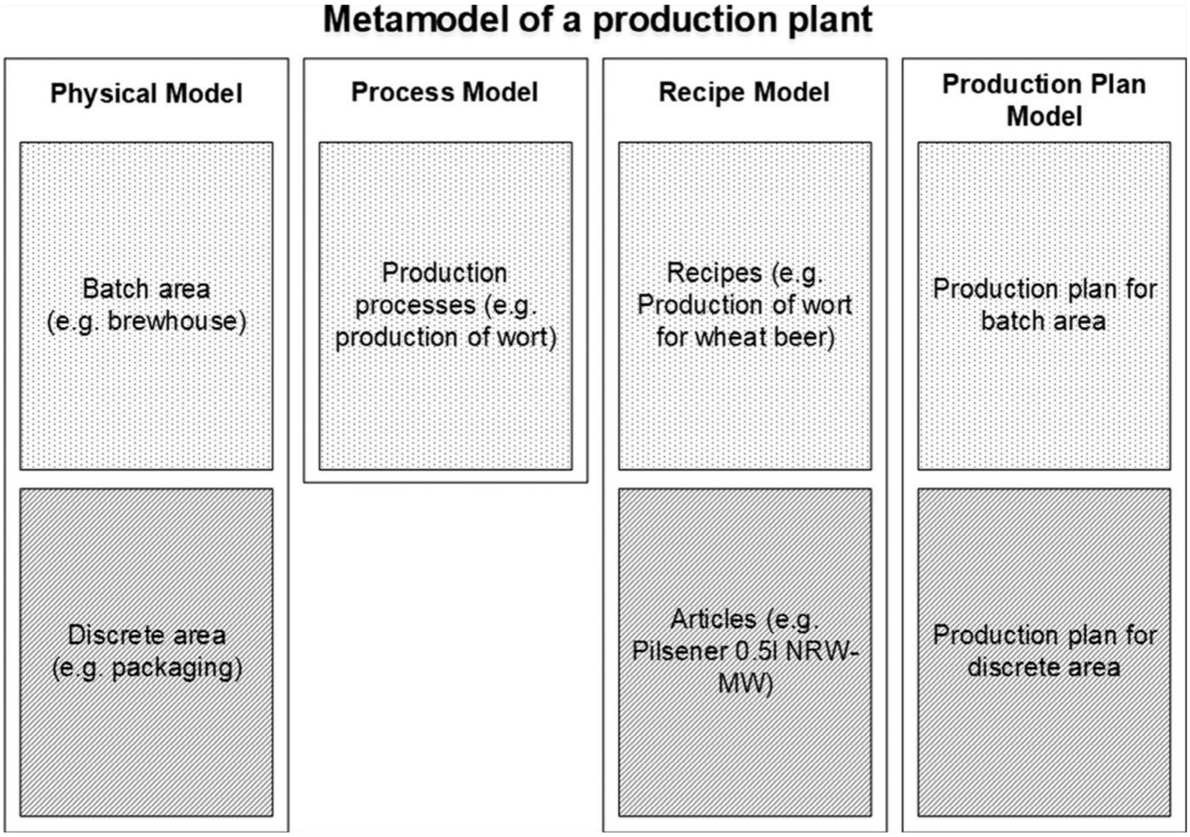


FIGURE 2 Structure of the metamodel for production systems (physical model, process model, recipe model, and production plan model); batch area (dotted areas); discrete area (dashed areas)

process cells as well as global framework conditions. The entirety of the models depicts a holistic production operation concerning all plants, processes, recipes, and articles, as well as the production plan.

4.1.1 | Physical model

The physical model follows the hierarchy of ANSI/ISA S88,[29] see Figure 3. Thus, at the top level, the class *Physical_model* comprises any number of *Process_cells*. Like the subordinate class *Unit*, this class has certain additional information such as specific IDs and identifiers. Any number of classes of the unit can be assigned to a process cell. Due to the different production methods and functions, there is a further subdivision into five different unit classes. These include *Batch*, *Discrete* and *Conveyor* units, as well as *BranchMerge* and *SourceSink units*. *Batch_unit* includes units that follow the batch-oriented mode of operation and have a process-dependent energy and media consumption. In addition to subclasses with further parameters, there are also the classes *Consumption_factor* and *Recuperation_factor*, which contain conversion factors for the consumption of energy and media as attributes. These factors are also used in the description of the process and recipe model and are described there in more detail.

The four remaining unit sub-classes associate *Simulation_parameter* in a composition. One object of the simulation parameters is the *Technical_data*, which varies in scope depending on the unit class. It represents the function of a unit concerning the mode of operation and parameterization of the material flow of the simulation. The *Output_value* describes the production speed of a machine, while the *Capacity* describes the units within a machine that are processed simultaneously. The *InOut_ratio* enables the specification of a packaging ratio of a machine, for example, the number of bottles within a secondary packaging. The attributes for *Sorting*-, *Stocking*-, and *Storage_behavior* enable the specification of product rejections, for example, by inspection machines, information on the processing method, or the storage behavior of units. Besides, the failure behavior based on the mean time to repair (MTTR) and the mean time between failures (MTBF), as well as the resulting availability is described in the class *Failure_behavior* [56]. The class *State_data* contains the consumption data (*Energetic_parameters*) for energy (electricity and thermal energy) and media (water, compressed air, CO_2) for the operating states Operating, Lack/Tailback, Failure, and Off.[27] This means that a specific consumption level for each type of energy and media is present at a certain operating state of a machine. *Article_dependency* enables, in conjunction with the recipe model, an article-specific specification of the simulation parameters including the subordinate classes. The unit class *BranchMerge_unit* describes the separation or merging of material flows and the unit class *SourceSink* describes the creation and

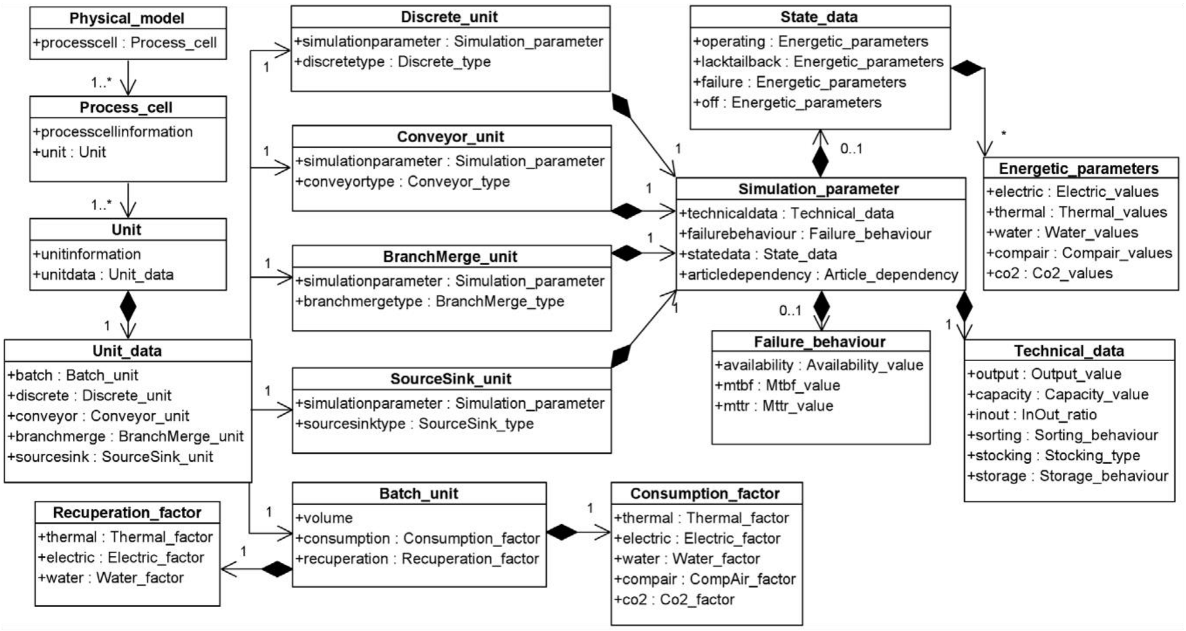


FIGURE 3 UML-class diagram for physical metamodel

destruction of material at the beginning or end of material flow. Both unit classes are essential for the function of a simulation.

4.1.2 | Process model

The process model, as shown in Figure 4, follows the hierarchy according to ANSI/ISA S88. A *Process_Model* can contain any number of *Processes*. Further attributes of this class are a name and an ID. The subordinate classes *Process_stage* and *Process_operation* are structured according to the same scheme. Since the *Process_operation* level has been defined as the energy-relevant level, further attributes are defined here. The sequence of the individual process operations is defined using *connections*. The *Process_operation_type* describes the function of the process operation, such as filling, processing, or emptying. The *Simulation_information* contains attributes such as time and the consumption values for all energy and media types for a process operation. The *Consumptions* describe the total requirements of the respective energy and media type throughout the *Process_operation*. Considering the *Recuperation_factor* for energy being reused and the *Consumption_factor* of a unit in the physical model, the consumption values can be calculated. This allows a process- and unit-specific description of consumption, whereas a process can be performed on different process cells of a production system. The sequence of arbitrary process operations with a specific consumption of energy and media allows detailed mapping of a consumption profile to a process.

4.1.3 | Recipe/article model

The *Recipe_model* (see Figure 5) covers all recipes, represented by a process and articles which can be run on process cells. The class of the *Recipe_information* has a *name* and an *id* as attributes. A *Process_stage* comprises the sequence of *Process_operations*. To be able to map the necessary flexibility of production in a brewery, process stages are assigned to units in the recipe model via the class *Process_stage_link*. This link results in the calculation of the consumption levels via the factors explained in Section 4.1.2. This offers the advantage, that the process model is independent of the physical model and enables multiple uses of a process for different units considering different consumption levels. Also, the class of the *Batch_parameter* contains attributes which describe,

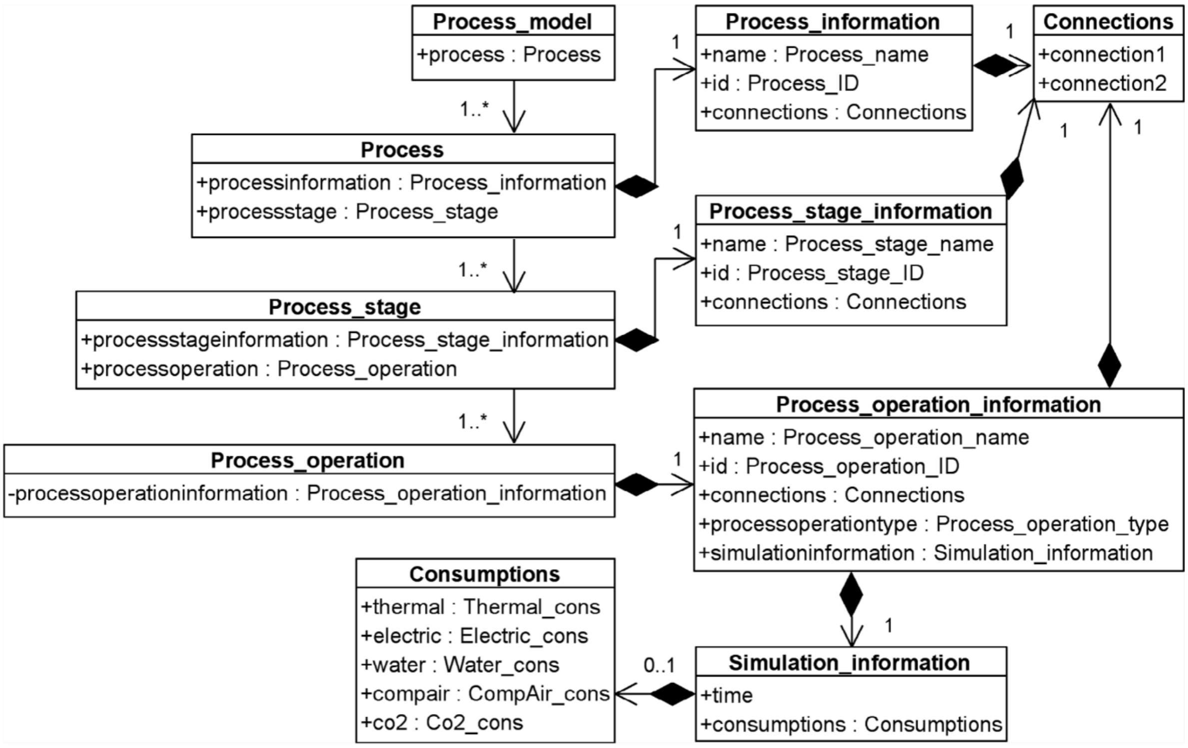


FIGURE 4 UML-class diagram for process metamodel

for example, the volume of the batch. The *Discrete_recipe* describes all possible articles that can be produced on process cells of the discrete manufacturing method and assigns them accordingly. Since different articles usually have different parameters for each unit, this had to be considered in the metamodel. This can be reflected in terms of all *Simulation_parameters*, such as operating speed, but also the consumption of energy and media. The linking of the respective article with a unit from the physical model is done through the class *Link_element*, in which all attributes of the respective *Discrete_unit* can be specifically adapted via a *Recipe_id*. Thus, the possibility of a global parameterization of a discrete unit, valid for all articles to be produced on it, as well as the specific parameterization with article-specific parameter sets, is guaranteed. In addition, the class *Packaging_parameter* contains further attributes relevant to the article, such as the packing ratios (see *InOut_ratio)* and associated dimensions.

4.1.4 | Production plan

The *Productionplan_model*, as shown in Figure 5, describes the chronological sequence of *Discrete_recipes* and *Batch_recipes* on physical plants and thus provides the framework conditions of a metamodel for the simulation of a production system. The *Productionplan* consists of three sub-models. Attributes with simulation-relevant parameters are also described in the class *Productionplan_information*. Since a production plant mostly does not operate around the clock, the class of the

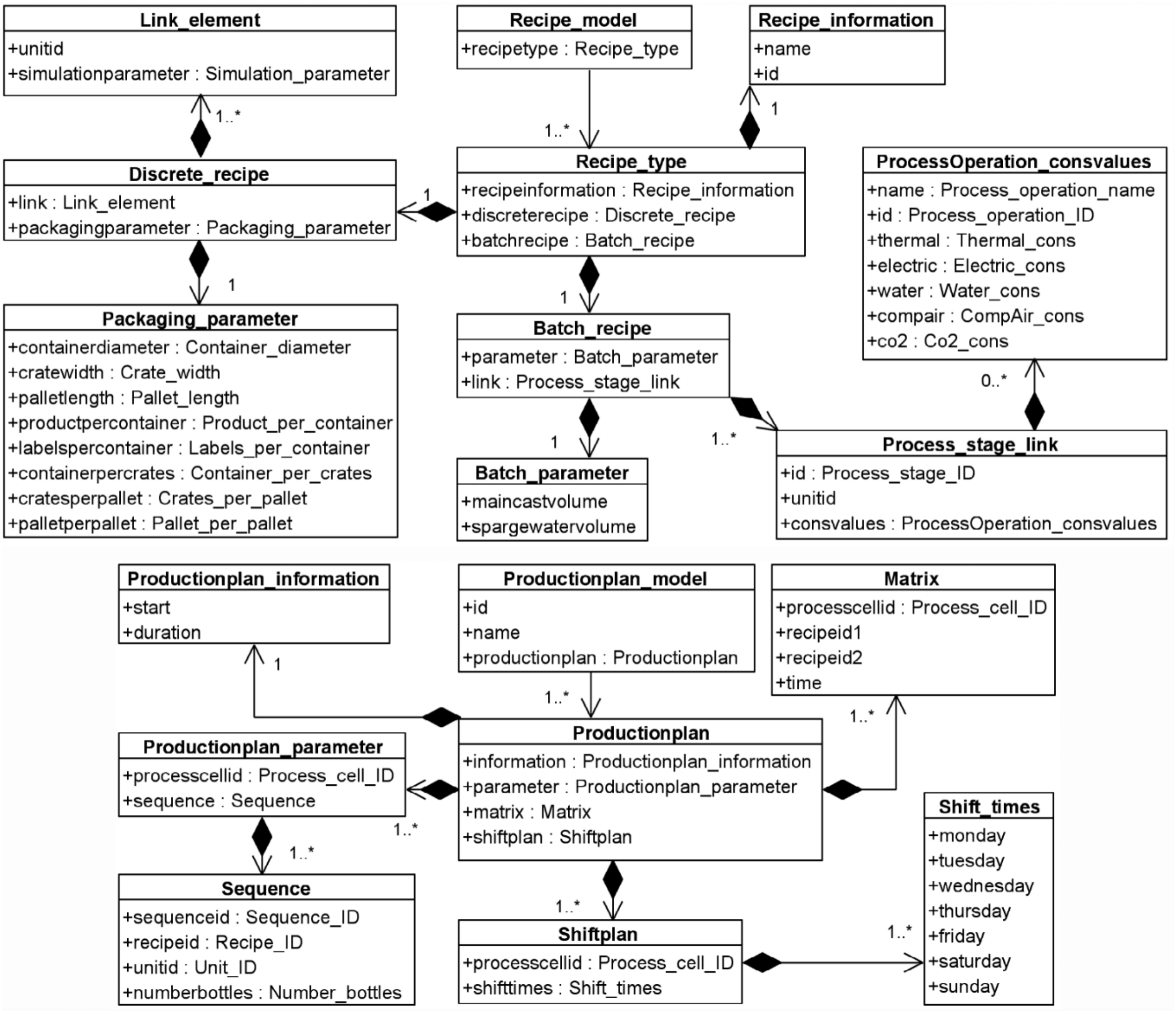


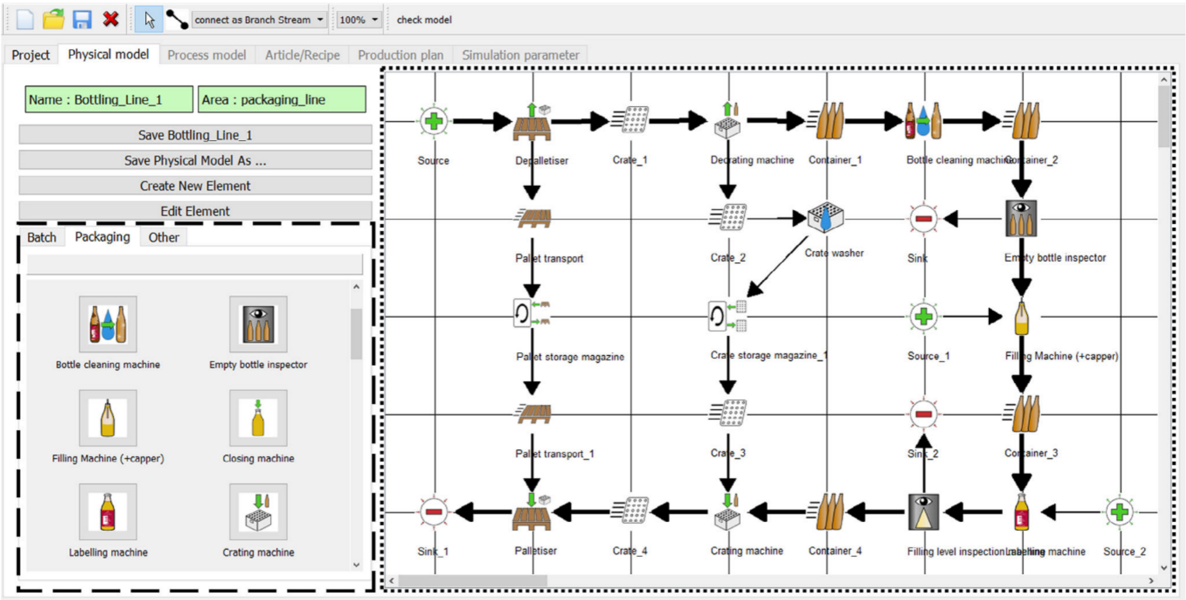
FIGURE 5 UML-class diagram for recipe and production plan metamodel

Shiftplan describes the possible working times for each process cell and each weekday. These limit the entire period by the planned nonproduction time. Outside this period, no production takes place. The chronological *Sequence* of recipes on a process cell is a special feature, as several recipes can be active at the same time. Since a unit can only process one recipe, the time sequence of the recipes plays an important role. The varying time interval between two recipes are represented by a class *Matrix* with the *time* intervals as attributes. The equivalent is the sequence of articles, where the time intervals between two articles on a process cell, are caused by changeover and cleaning times. The *Productionplan_parameter* represents the third pillar of the production plan model. In this model, the sequence of recipes or articles assigned by the attribute *Sequence_ID* is defined in the class *Sequence*. The assignment is made using the *Recipe _ID* and the superordinate *Process_cell_ID*. As a result of the three models in the production plan model, the *Simulation_parameter* of the source unit of the physical model is parameterized, depending on the framework conditions.

4.2 | Development of a modeling solution

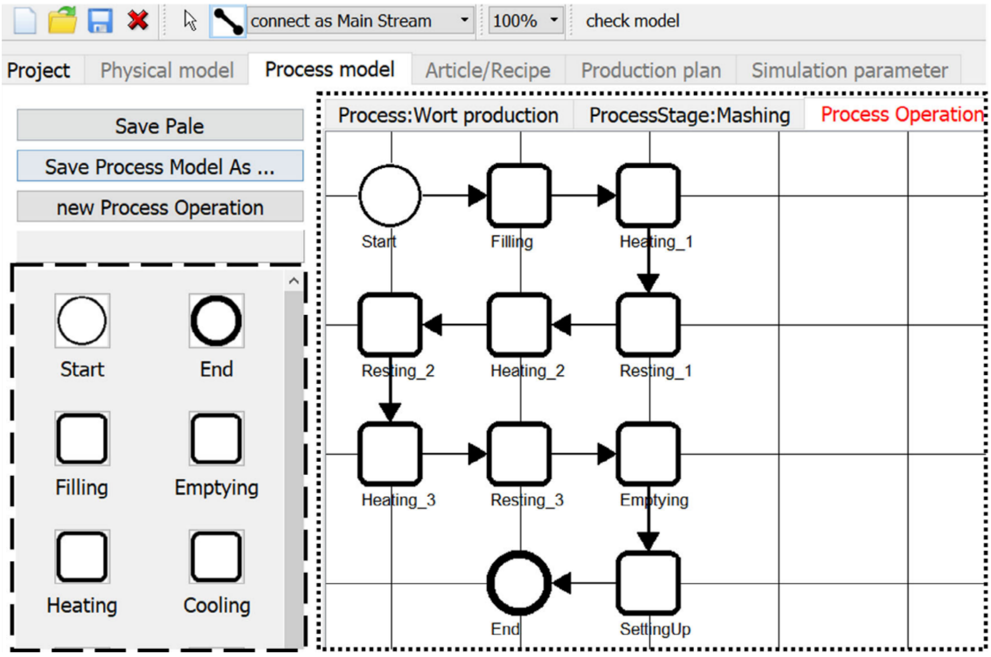
The main aspects of the requirements for the software solution result from the identified barriers and challenges for the manufacturing industry, especially for SME, as well as the scientific gap. Thus, they are simple, fast, and context-free modeling possibilities, which do not require any prequalification in the field of modeling and simulation. For an intuitive handling, the software solution should be able to represent the full potential of the metamodel in terms of level of detail of the models and flexibility. As real use-cases and for testing, two different brewhouses for the batch area, as well as two returnable-glass bottling plants for the packaging area were modeled in the editor. In addition, the associated recipes, articles and a production plan were also modeled. Excerpts of these are shown in Figures 6 and 7. The developed modeling editor is a platform-independent software and is structured in individual modeling columns according to the metamodel. The modeling editor has a start interface that provides an overview of the model of a production plant and offers the possibility of loading and saving it in form of an XML file. Starting from this interface, models of the four modeling columns can be created. All models can be copied and edited, which simplifies a later experimental procedure during the simulation. The modeling of the physical model is based on the modeling language MES-ML[49] and depicts the plants and machines of the unit level, according to ANSI/ISA S88.[29] The model creation is carried out via block libraries, in which, depending on the areas of batch plants, packaging machines and others, the most common units in the brewing industry are stored. Using the drag-and-drop principle, the blocks can be selected and placed on a modeling surface, behind which a coordinate system is stored. With the help of connections in the form of arrows, the physical connection of the building blocks can be established, partly with the distinction between main product flow and side flow. A further parameterization of the individual blocks is carried out according to the metamodel presented in Section 4.1.1. It is also possible to differentiate whether the respective parameters are global, that is, valid for all articles produced on this unit. Otherwise, an article-dependency of the parameter can be specified and the further parameterization takes place in the article model. In order to offer the greatest possible flexibility with regard to plants and machines to be depicted, the user has the possibility to define blocks himself or to adapt existing blocks. However, this requires deeper process knowledge. Figure 6 shows the physical model of a real returnable-glass bottling plant in the editor, as described in Section 2.1. In addition, another bottling plant, producing PET-returnable bottles, was modeled. The two plants differ on the one hand in the type of machines used and in the installation of the plant, and on the other hand in the articles to be produced. Especially the different types of containers and packaging, but also production types (e.g., new container feed, use of a tunnel pasteuriser, use of a flash pasteuriser or a mixer) for the respective articles could be mapped. In the batch area a brewhouse according to Section 2.1 was depicted. A second brewhouse including an alternative boiling system using a buffer tank, a booster for heating up and a gentle cooking system by using a thin-film evaporator was modeled.

The modeling of a process model is done according to MES-ML, as described by Weissenberger et al.[49] This modeling language is based on the Business Process Modeling Notation. The modeling of the process model is equivalent to physical modeling and represents the structure of the process according to the ANSI/ISA S88.[29] The modeling starts at the process level. To determine the desired sequence of the individual process steps, the start and end must be defined with the help of an element. The processes are linked using connections. This procedure runs through all levels. By selecting a process, for example, it can be deepened and the process stages can be modeled. The selection of elements is made by predefined processes, which are stored in a block library. Since the level of process operations has been defined as energy-relevant, the further parameterization of times



Name : Bottling_Line_1
Area : packaging_line

FIGURE 6 Modeling of a returnable-glass bottling plant for a physical model in the modeling editor (left: block library (dashed); right: modeling surface (dotted)); the parameterization of the machines is carried out by special input masks



Process:Wort production
ProcessStage:Mashing

FIGURE 7 Modeling of a process model (process operations for the process stage "mashing" (left: block library (dashed); right: modeling surface (dotted)))

and consumption values is done here. It is possible to extend the process block library at will and thus adapt it to the specific needs of the user. A process operation model always starts with the filling of a unit, followed by a processing part (e.g., heating and resting). After the latter it is emptied. Subsequently "setting up" process operations can be defined. Figure 7 shows the process model on the process operation level for mashing in the editor.

The parameterization of the process operations is carried out by special input masks. For validation different types of mashing processes were modeled. On the one hand an infusion mashing process, just using the mash tun, is modeled by stringing together a sequence of heating and resting process operations. On the other hand, a decoction mashing process, including a mash pan, where a part of the mash from the mash tun is cooked, could be modeled by customizing the sequence of process operations. Furthermore setting-up processes, for example, in the lauter tun, after lautering, like the removal of brewers spent grain and the following rinsing, can be depicted by adjusted process operations, which can take part after the emptying of a unit.

The modeling column for recipes and articles comprises the third column of the modeling editor. This is depending on whether it is a recipe, which links a process of the process model with a process cell of the physical model, or an article, for which packaging machines of a process cell can still be parameterized. Thus, when creating a recipe, all possible batch units of all process cells, as well as all process stages of the processes, are listed and can be linked to each other by marking and confirming. In this way, it is determined for the later simulation which process operations are performed on which unit. Also, the corresponding energy levels, consisting of the consumption data of the process, and the consumption factors of the respective plant, are calculated. This allows maximum flexibility in combining recipes with different production lines. When creating an article to be filled, the parameters for describing the article on the one hand and article-dependent machine parameters on the other hand are in the foreground. To counteract the problem of the numerous parameters required for each packaging unit, multiple optimizations were implemented. For example, by specifying the packaging ratio (e.g., the number of bottles per crate) as well as the container dimensions, the grouping behavior of the units, and the size of the container and container buffer sections are automatically calculated. As different filling articles have different parameters, such as machine speeds and consumption values, due to their containers and the product itself, this must be considered in the modeling editor. For this reason, it is possible to parameterize each unit parameter specific for the current article. Therefore, the same input masks for the parameters as in the physical model are used.

The modeling of the production plan is carried out via the three sub-models as presented in the metamodel. To limit the total time to the plan occupancy time, the working hours for each weekday can be defined in tables for the shift model for each process cell. This data can be taken from the shift plan of the production plant. Outside these times, no production takes place. A production schedule can be defined for each process cell. A distinction is made between production schedules for both areas of the physical model. In the batch production plan, a sequence of recipes that are to be produced on the process cells in the simulation can be created. With the help of a matrix to be defined, which reflects the brewing sequences, the duration between the starts of the individual recipes can be determined. A changeover/cleaning matrix is used to create a production plan for articles. When individual filling orders are created, the number of articles to be produced in the simulation can be varied.

Finally, general information concerning the simulation, such as start and duration, are determined. When determining the start time, the day of the week is also specified. This enables a realistic production plan, as production-free weekends can be mapped. When exporting the model of a production plant, all relevant elements, and parameters are exported to an XML exchange file. To increase the usability of the software, further features were implemented. For this purpose, a help menu was created, which covers all features of the software. It contains explanations about the functionality of the software, all modeling approaches as well as for the specific adaptation of the editor. Additionally, for better error localization and to ensure the correct simulation of the models, an automatic check of the models for correctness and completeness is implemented.

The modeling software developed can be executed in Microsoft Windows runtime environment, regardless of the end device. Mouse and keyboard, but also touch solutions can be used as input devices. Besides the user, the only other interface is the presented XML file. This file is used for export, but also for saving the models. Concerning the required CPU power as well as the main memory, no special requirements are set and can be neglected. The software can be executed by simply starting an executable file, no installation, even of additional software, is required. The total size of the software including all required files is 20 MB. The source code in C++ comprises 43 000 lines. The maintenance and service of the software can be carried out by qualified personnel using the open-source development environment Qt. During the development phase, ongoing verification, as described by Reference,[51] of every part of the software solution by several parties took place.

4.3 | Validation of the modeling approach and modeling editor

For the answering of the questions in the questionnaire for the validation of the modeling approach and modeling editor, a German school grading system, whereby a grade of one means very good or full agreement with the question and a grade of six means insufficient or full rejection, was used. The main findings, in particular with regard to the four criteria, are presented in more detail. One of the most important questions regarding the comprehensibility of the modeling approaches is primarily aimed at the metamodel based on the four modeling pillars. The implementation in the modeling approach should make the metamodel easily understandable and comprehensible. Accordingly, the rating of the *Comprehensibility* with an average of 1.8 turns out to be good. The comprehensibility and traceability of the physical and process model were rated "good", with an average of 1.5. The test persons, who already had previous experience with modeling, also stated that the modeling approach definitely facilitates modeling with regard to simulation and they can imagine using the modeling in the future. The test persons see a need for improvement in the intuitive navigation through the modeling editor (average of 2.25). The modification possibilities of the systems, processes and parameters were evaluated as "good" with regard to speed and simplicity as well as the possibility of article-dependent parameterization. The *Simplicity* of using the entire modeling editor without specific prior knowledge in the field of modeling and simulation of production systems was rated "good" with an average of 1.8. The test persons also rated the *Completeness*, that is, the coverage of an entire production system by the modeling approach, as "very good" with an average of 1.4. Finally, the *Sustainability* of the modeling approach and the modeling environment, that is, the use of the methodology for other production industries, was rated as "very good" with an average of 1.25. In addition to the evaluation of the questionnaire, the XML file created by the test persons was also checked for correct modeling and simulation capability by using the presented check function.

4.4 | Potential applications of the metamodel and simulation studies

The creation of simulation models for a forecast of the energy and media demand of a production system can certainly be done without a metamodel. Nevertheless, numerous use-cases for simulation experiments describe the necessity of a metamodel. Since the metamodel has a generic and hierarchical structure, existing models can easily be extended and adapted. In case of planned investments, models provided by the plant manufacturer can be implemented into an existing model and the energetic impact on the production system can be verified by simulation in advance. The metamodel also provides the amount of data and parameters required for a simulation.

A precise estimation of the energy and media requirements in advance also plays a major role in the design of the supply facilities. The metamodel supports the mapping of peak loads by means of the defined consumption behavior of the different working units. Especially the avoidance of these peaks, for instance by adjusting the production plan, offers potential for improving energy efficiency. The generic and context-free metamodel allows a flexible simulation regarding the level and depth of the simulation, which depends on the objective of the simulation experiments. Thus, entire production plants or only parts of process cells can be simulated. In addition to a detailed, article- and recipe-specific consideration of a system to uncover optimization potentials and determine influencing factors, the metamodel also allows a global analysis. This is, for the first time, enabled by the metamodel concerning both production areas as well as all types of energy and media. Thanks to the ANSI/ISA-S88 standardization it can be applied to a large number of companies in the beverage industry. This creates uniform comparability and allows benchmarking.

In order to demonstrate the suitability of the modeling approach and the editor, two simulation studies were carried out. The modeling examples described in Section 4.2, a brewhouse and a beverage bottling plant, form the basis of the simulation studies. The time-discrete simulation software "PacSi," which masters the simulation of packaging processes,[57] was used. The software was extended to the simulation of batch-oriented operation as part of the development of the entire methodology. In addition, numerous functions, such as automatic model generation through the assignment of building block elements, were implemented. A broad base of measurement data, from which the simulation-relevant parameters were determined, was used. The simulation models were generated automatically in a simulation environment and the results were issued numerically and graphically with the aid of specially programmed evaluation tools. The brewhouse of a medium-sized brewery was modeled in the modeling editor with the existing units, including different processes and recipes, and considering a real production plan (see Section 4.2). The goal of the simulation study is to reduce the peak loads of the thermal energy demand by slightly adjusting the times between the individual brews of the recipes (see Section 4.1.4: Matrix, +time). The simulation duration covers a period of 7 days in which a total of 71 batches of three different recipes are produced. Figure 8 shows a section of the comparison between the thermal energy demand curves of the brewhouse before and after the adjustment of the brewing sequences. In the simulation, it was possible to

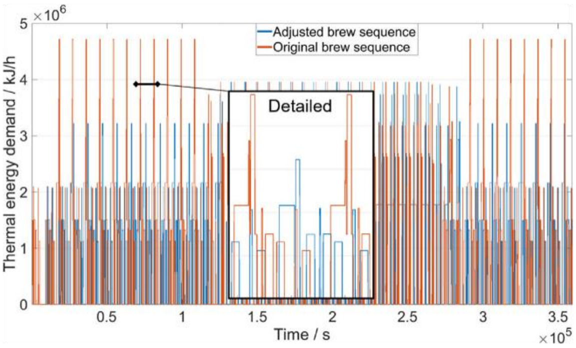


FIGURE 8 Comparison of the curves of the thermal energy demand of the brewhouse in the original and adjusted brew sequence (section)

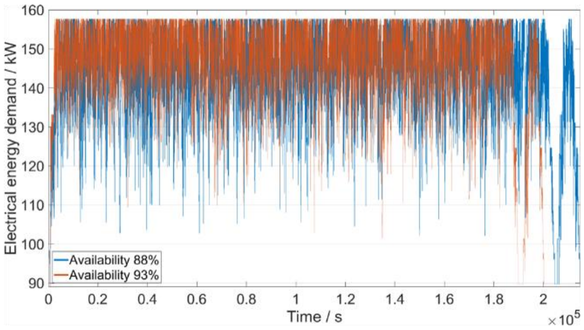


FIGURE 9 Comparison of the curves of the electrical energy demand of the beverage bottling plant at an availability of 88 and 93%, respectively

reduce the peak loads of the thermal energy demand by 32%, especially for the first recipe.

Furthermore, a returnable-glass bottling plant (see Figure 6) was modeled in the modeling editor. Two filling articles, each with article-specific parameters and a production schedule with a duration of 62 h were modeled. The aim of the simulation study is to investigate the influence of plant availability on the energy and media requirements of the beverage bottling plant. For this purpose, adjustments were made to the MTBF (Failure behavior; +mtbf) of the individual units using the modeling editor, resulting in an increase in plant availability of 5% (to 93%). The simulation was carried out with a repetition of n = 10 trials. In addition to the savings in electrical (4.25%) and thermal (4.01%) energy as well as compressed air (3.11%) and CO_2 (6.5%), an accelerated production of approx. 3.5 h (6.4%) was determined as a result of the increase in plant availability. An increased water consumption (5.32%) can be ascribed to the fact that the bottle cleaning machine was in the "Operating" state, which significantly increased consumption, for a longer period of time. Figure 9 shows the course of the electrical energy demand of one simulation run of the corresponding parameterized availability. The change-over and production of the second filling article toward the end of the simulation run can be seen. Production ends noticeably earlier at a plant availability of 93%. Due to the stochastic failure behavior of the individual units and the resulting energy levels, the fluctuating course of the electrical energy requirement results.

5 | DISCUSSION

This publication aims on developing a hybrid modeling approach for the context-free representation of a production plant in the beverage and brewing industry for the prediction of energy and media consumption. Based on this approach, a modeling environment was created, which should allow modeling without specific previous knowledge as well as fast and easy model generation. This should enable SMEs in particular to overcome their barriers and optimize their energy efficiency. The challenge in the development of a modeling approach for the representation of an entire production plant for energy and media simulation is the definition of clear system boundaries and necessary information to be able to make forecasts as accurately as possible later on. Strict adherence to and the implementation of the ANSI/ISA S88 standard, which describes the subdivision of production systems into several pillars, provides the basis for standardized and context-free mapping. In combination with the hierarchical subdivision of the columns, flexible horizontal and vertical model granularity is also enabled. This means that not only the depth of the model, but also the scope of the model of a production plant can be varied. This provides maximum flexibility in the application of the metamodel. In order to evaluate the metamodel with regard to these points, some models have already been created after the implementation in the modeling editor. Thereby the brewhouses of two medium-sized breweries were mapped. The differences are also reflected in changed processes and thus recipes. Two reusable beverage bottling plants with different articles to be produced have also been shown in the packaging area. The possibility of process and article-dependent parameterization of the recipes or articles allows a very precise parameterization of the model. In any case, the metamodel was suitable for mapping all variants and contents the information required for a model to investigate energy and media requirements. This represents the main challenge in model creation, since the data basis in the production plants is usually very small and the development of the parameters is complicated and time-consuming. The advantage of converting the metamodel created in UML into an XSD is that the XML file resulting from the modeling environment, which describes the model in detail, can be validated against the schema. This means that the schema can be used generically as a check for all created models. In addition, the structure, semantics and data types defined in the schema can be used as an aid for the required mapping in any simulation environment for the automatic generation of simulation models. Up to now, no sensors and interfaces that transfer simulation-relevant data and parameters to the software solution have been connected and implemented. It is conceivable that in the future this will be delivered automatically by machines via suitable interfaces, such as the Weihenstephan Standards, or directly by the machine manufacturers. The metamodel was implemented in a software solution and should offer the possibility to create inexpensive simulation models quickly and easily. Due to the platform independence of the software it can be used on any device. The strict implementation of the metamodel by mapping the hierarchical modeling columns allows context-free and generic hybrid modeling. The modeling environment was continuously verified against the XSD during the development period and after completion it was validated by a systematic test by test persons with respect to the mentioned criteria. The comprehensibility of the models and its representation in the modeling environment was rated as good. This is because models are independent and context-free of each other and are created in the individual modeling domains. The difficulty here is to convey an understanding of the interconnection of the individual modeling pillars. The testers included people who have no previous knowledge of modeling and simulation. The simplicity of the modeling environment was also rated as good. The numerous aids and simplifications within the modeling editor play an important role here. Starting with the help menu, which describes the handling as well as all elements in detail, the function of the automatic checking of models is also an essential point for the easy and fast creation of working models. Furthermore, simplicity is increased by the graphical modeling in the area of the physical model and the process model, based on predefined block libraries. Parameterization is facilitated by, for example, the specification of packaging material ratios and the automatic calculation of the resulting parameters or buffer capacities for different articles. Nevertheless, the validation revealed numerous possibilities for improvement regarding the operation of the modeling editor, which were categorized and implemented accordingly. The completeness of the modeling approach is, especially for nonexperts, a difficult factor to evaluate, as it depends on the specific task. Therefore, clear system boundaries were defined and some use cases were described before the entire methodology (development of a modeling approach and a simulation environment) was developed. This was explained to the respective test persons and they were asked to give an estimation. This overlapped well with those familiar with the methodology and was rated as very good. The determination of the simulation granularity on the unit and process operation level plays a major role. Although coarser modeling would be simpler and much faster, many aspects of a simulation of a production system, such as load peaks in consumption, would be lost. More detailed modeling would provide better simulation results but would require an enormous effort in parameters, which contradicts the requirement of fast and simple modeling. The sustainability criteria describe the generosity of the modeling approach and its application to other production industries and were also rated as very good. The essential prerequisite for this is strict compliance with existing standards, such as ANSI/ISA S88. The modeling editor offers a good possibility to adapt the software solution to other industrial branches by adapting block libraries and easily creating specific blocks.

Furthermore, the simulation studies provided an initial insight into the entire methodology, from modeling to simulation experiments. The case studies show that the metamodel is suitable for representing brewery production plants and forming the basis for an executable simulation model. The challenge here, depending on the complexity, is the parameterization of the models. The simulation studies refer to a detailed and extensive basis of data. In both cases, energy and media savings could be achieved in the simulation by adjusting parameters via the modeling editor. This shows that the modeling approach is very well suited for a fast and simple analysis of plants in the beverage industry. The modeling editor represents the interface to the simulation environment. Simulation models can be generated automatically based on the XML exchange file.

6 | CONCLUSION

It can be concluded that the modeling approach is suitable for mapping an entire production about the simulation of energy and media consumption. The advantages and possibilities of the presented metamodel are:

Structured, hierarchical, and generic modeling of an entire production system in terms of energy and media requirements.
Context-free and therefore flexible modeling columns.
Mapping of batch-oriented and discrete operation as well as dependent consumption behavior in one model.

Creation of the basis for the data and parameters required to forecast energy and media consumption.
Application of the modeling approach to other industries by implementing the ANSI/ISA S88 structure.

The suitability of the metamodel was able to be demonstrated by means of use cases as well as simulation studies. A possible solution for SMEs is the developed modeling editor, in which the metamodel was implemented. The context-free modeling in the four modeling pillars is easy to understand and can also be carried out by nonexperts. Graphical modeling with block libraries and numerous aids for the user ensure simple and fast model creation. This could be validated and proven by a systematic test. The structure of the XML exchange file, which is described in a schema file and which represents the result of the modeling editor, allows a favorable simulation model creation since this can be realized in any simulation environment. On the basis of two simulation studies, it could be shown that executable simulation models can be generated on the basis of the metamodel and the energy and media consumption behavior can be represented. Based on the findings, the following objectives can be defined for further work. The authors will present the automatic simulation model generation in a simulation environment in detail. The simultaneous simulation of both operating modes, batch and discrete, at the same runtime will be a novelty. In addition, an entire production system in the brewing industry is to be simulated with regard to its energy and media requirements. The required data basis represents a challenge. A standardized measurement concept and evaluation procedure, considering existing approaches, could provide a remedy and could also be easy to apply. Therefore, the authors will discuss an approach to determine the simulation parameters in both areas of the brewery. To prove the suitability of the entire method, a detailed validation will be performed using real measured data. Furthermore, extensive simulation experiments with a wide variety of approaches, such as the modernization of plants or the adjustment of the production schedule, to reduce the energy and media demand are planned and will be addressed in further publications. The goal of the whole methodology is to create the possibility for a quick and easy analysis of entire production plants in the brewing industry about energy and media consumption and this will offer SMEs in particular an opportunity to optimize their production.

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CONFLICT OF INTEREST

The authors declare no conflict of interests in this research.

AUTHOR CONTRIBUTIONS

Raik Bär: Conceptualization; data curation; formal analysis; investigation; methodology; software; validation; visualization; writing-original draft. **Tobias Voigt:** Conceptualization; funding acquisition; project administration; supervision; writing-review & editing.

DATA AVAILABILITY STATEMENT

Author elects to not share data.

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2.3 Publication III – Automatic model generation and simulation of the discrete bottling area of the brewery

Bär, Raik; Zeilmann, Michael; Nophut, Christoph; Kleinert, Joachim; Beyer, Karsten; Voigt, Tobias. **Simulation of Energy and Media Demand of Beverage Bottling Plants by Automatic Model Generation**. Sustainability 2021, 13, 10089; DOI: 10.3390/su131810089

Environmental challenges, high energy costs, and growing public awareness are challenging the global brewing industry to produce sustainably and efficiently. The filling and packaging of beverages, which are characterized by complex interrelationships and diverse machinery as well as a high share of the total energy demand of the plants, is a particular focus of attention.

This paper presents a novel method for the prognosis of energy and media demand of beverage bottling plants. Based on the previous presented modeling approach a holistic automatic simulation model generation from a configuration file in a simulation environment is developed. For the determination of measurement data, a generic and standardized data structure is introduced. In combination with an automatic simulation parameter determination method, the relevant parameters for the holistic representation of article-specific production on beverage bottling plants can be determined. A beverage bottling plant was studied in detail and a comprehensive model could be created. An extensive validation was carried out based on two validation periods in a unit-specific way and especially focused on the electrical energy demand and the consumption of compressed air. It was confirmed that the method is capable of a realistic representation of the energy and media demand of beverage bottling plants and was furthermore applied for two use cases to increase the energy efficiency. The approach enables the uncovering of potential savings, the testing of the effectiveness of optimization strategies as well as a support for possible investment decisions.

Contributions of the doctoral candidate (CRediT):

Conceptualization; methodology, software, validation, investigation, writing - original draft, visualization, project administration;

sustainability

MDPI

Article

Simulation of Energy and Media Demand of Beverage Bottling Plants by Automatic Model Generation

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Abstract: Facing environmental challenges, high energy costs and a growing public awareness, the global brewing industry is increasingly publishing ambitious targets toward a more sustainable production. Small and medium-sized enterprises of the brewing and beverage industry cannot ensure energy and media efficiency mainly due to capital and knowledge inadequacy. This article addresses this problem and presents a pragmatic method to determine the energy and media demand. Accordingly, a modeling editor as well as a standardized data structure and automatic simulation parameter determination tools were developed to implement the method. A given production plant can be modeled with adequate details using the presented editor. Based on a configuration file, a holistic simulation model can be generated automatically in a simulation environment. A beverage bottling plant was studied, and the necessary datasets were obtained for implementing the proposed editor and, thereby, the method. It was confirmed that the simulated values of electrical energy and compressed air consumption match the measured empirical data. The measures to increase energy and media efficiency were also found effective. Using the presented method, enterprises of the brewing and beverage industry can easily uncover avenues for potential savings, test the effectiveness of optimization strategies, and substantiate possible investment decisions.

Keywords: bottling; modeling; simulation; energy and media demand; validation

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1. Introduction

For a clean and sustainable production, the brewing and beverage industry is challenged to optimize its energy efficiency [1]. Facing environmental challenges, high energy costs and a growing public awareness, including the United Nations sustainable development goals [2], the global brewing industry is required to produce more sustainably. Large brewery groups, in particular, publish ambitious targets regarding a more sustainable production [3–5]. When discussing sustainable production, different issues, which should be considered at the same time, must be taken into account [6]. In addition to the material efficiency of the materials of the primary production, energy efficiency plays a particularly important role [7,8]. The material efficiency requires knowledge of the previous production processes. With the help of a simulation, which is also mentioned as a tool for optimization in the course of the digital factory [9,10], the energy efficiency can be improved [11]. The simulation is primarily used for the holistic analysis of complex production systems and is suitable for uncovering the optimization potential without interrupting the ongoing production [12,13]. The beverage industry is challenged by the conflicting demands of high product quality and diversity and cost-effective production. Increasing energy efficiency and flexible production can sustainably reduce costs and consequently increase competitiveness [14,15]. However, simulation studies are usually associated with high costs and require a high level of expertise, especially for modeling complex systems [16]. In addition, a comprehensive database is essential for the success of simulation studies [12].

However, these data are subject to uncertainty. This presents insurmountable barriers for a sustainable production for small and medium-sized enterprises (SME) [17,18]. The beverage industry, whose production is very energy- and media-intensive [1], is characterized by small companies: 90% of the German brewing landscape consists of small and medium-sized breweries [19]. About 30% of the electrical energy demand and about 25% of the thermal energy demand can be attributed to bottling/packaging [1,12]. Accordingly, this complex and multi-layered area holds a potential for increasing energy and media efficiency. Osterroth et al. [20] provides a detailed overview of the consumption structure in beverage bottling plants.

An overview of the simulation and other methods for increasing energy efficiency in batch-oriented processes and the discrete packaging area in the beverage industry is given by Bär and Voigt [12]. Publications in the bottling area consider a wide variety of aspects [21–24], mostly with a focus on increasing efficiency, but not on energy and media consumption [25–28]. Approaches considering an increase in energy and media efficiency are limited with regard to various factors. To enable simple, quick, and cost-effective analyses and optimizations for SMEs, these barriers must be overcome.

To map real behavior, the entire beverage bottling plant, with its interlinkages, must be considered [29]. Few approaches deal only with partial areas or machines or selected types of energy and media. Dilay et al. [30] describe the detailed optimization of a tunnel pasteurizer by investigating the energy impact of various input parameters. As a result, various concepts were presented regarding a structural modification of the machine to achieve considerable savings of thermal and electrical energy. In their green brewery concept, Muster-Slawitsch et al. [31] describe the increase of energy efficiency and the use of renewable energy sources in the brewery—inter alia, in the bottling area. The reuse of thermal energy through hot water management is investigated and optimized. The simulation of water flows in a dairy is used by Marchini et al. [32]. The impact of the plant layout on water consumption is investigated using two use cases, and savings of 7.2% are achieved in theory. Using the integration of life-cycle assessment in a discrete-event based simulation, Johansson et al. [33] simulate an aseptic packaging line for fruit juices. The entire plant is examined in terms of its emissions and waste, and a validation is carried out by comparing with real consumption values. It is shown that discrete-event simulation is a suitable tool for the rapid and cost-effective estimation of optimizations.

The complexity of the methods poses another challenge with respect to their ease of use. Hubert et al. [34] present a simulation based on reference networks. An approach for optimizing wastewater production by scheduling processes in a beverage bottling plant is presented. Compared to a genetic algorithm approach, 10% of wastewater could be saved and water demand reduced accordingly. A validation based on real data is not carried out, which is another cornerstone of the approaches described in the literature. Furthermore, water consumption is simulated with regard to chemical oxygen demand, a criterion of water quality [35]. A validation with real data shows the good fit of the simulation. Based on an extensive database, Osterroth et al. [36] analyzed the electrical energy consumption of the machines at a beverage bottling plant in detail. The operating state depended on the consumption behavior of the individual units and is proven, and time-dependent consumption levels within the states are introduced. An extensive validation underpins the method, which, however, covers only electrical energy. Forster [37] describes a holistic approach to the modeling and simulation of beverage bottling plants with regard to energy and media consumption. The discrete-event simulation environment Plant Simulation is used, and a model is represented by predefined components. Various energy and media consumptions are machine-specifically simulated using state models, and the results are outlined by way of example. However, no detailed insight is given into how energy and media consumption are mapped. The validation is also insufficiently presented and does not provide any information about the suitability of the method. Information on the framework conditions, such as the production process, is not given. The inclusion of a production plan enables a description of the energy consumption during inactive production times [38]. Hubert [39] describes in a comprehensive work a simulation based on reference networks of a beverage bottling plant over a period of one week regarding the electrical and thermal ernergy demand as well as the water consumption. The failure behavior of certain aggregates of the plant is described by a Weibull distribution for the operation and the failure, and, furthermore, the start-up as well as the production and the final phase of the bottling process are described. It is shown that the bottling area is one of the main consumers of the above-mentioned energy and media types and therefore represents an enormous potential for improving energy and media efficiency. Simulation studies for the entire brewery, based on the variation of production schedules by adjusting the start times of the respective recipes, were carried out to reduce the electric peak loads. Savings in the double-digit percentage range were achieved. The work describes an interesting holistic approach, whereas no validation with real data takes place. To overcome the mentioned barriers, user-friendly modeling and the automatic generation of simulation models are recommended.

However, the available database, which is usually insufficient, poses a challenge, in particular for validation [40,41]. There are numerous applications for validating simulations, such as the comparison with other models or with recorded data [42]. The choice of the appropriate validation technique depends on the degree of subjectivity [42,43]. Osterroth et al. [36] use the average percentage deviation (APD) and Theil's inequality coefficient (TIC) for the statistical validation of the simulation results, which tests the credibility of the model. This method is also used in some other publications [44–47]. Al-Hawari et al. [25] and Johansson et al. [33] both use the simple comparison of simulation results with the results of reality for the validation of their model.

The barriers listed are taken up in this work, and a method for the automatic generation of simulation models for the holistic simulation of energy and media consumption for beverage bottling plants is developed. Figure 1 shows an overview of the approach in its major steps. For a simple and fast modeling of complex production systems, an already presented modeling concept, implemented in a user-friendly software, was used [48]. With an extensive database, it was possible to model and parameterize beverage bottling plants with regard to the physical plant, the articles, and the production plan. The simulation model is automatically generated via an extensible markup-language (XML)-based configuration file in a time-discrete simulation environment. A holistic production plant with regard to all energy and media demands, including a production plan, could be simulated. The methodology is validated in detail and use cases are applied in this work.

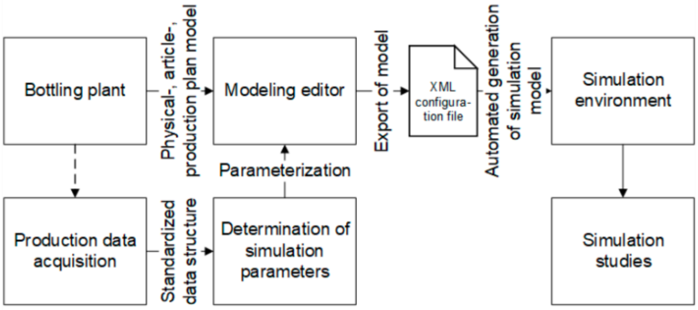


Figure 1. Overview of the main steps of the approach.

2. Beverage Bottling Plant Investigated and Database

The subject of the study is an industrial refillable glass beverage bottling plant for mineral water and soft drinks of one of the 10 largest mineral water companies in Germany (according to sales) [49]. The main product of the plant includes mineral waters, which are distributed nationwide. The plant is shown in simplified form in Figure 2 and generally represents the schematic structure of this type of plant. The plant is divided into three sections, depending on the transport equipment used (pallets, crates, and containers). The interlinking of the conveyors enables the buffering of downtimes caused, for example, by the failures of individual machines. If the buffer time of the conveyors is exceeded, downtimes lead to failure propagation, which is characterized as a lack or tailback situation.

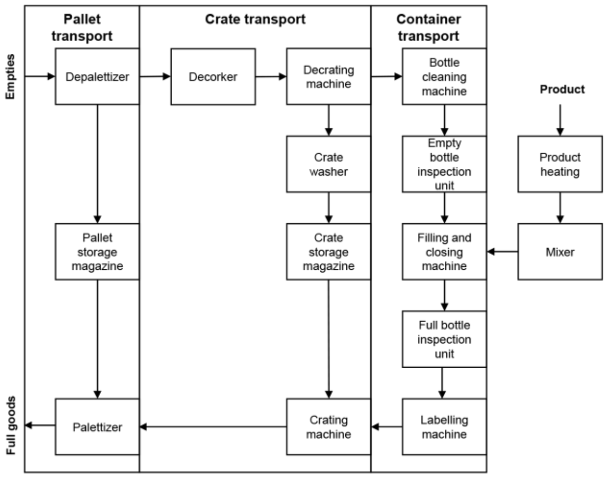


Figure 2. Schematic of the beverage bottling plant investigated.

The empties are brought into the plant on pallets, and the crates are destacked by the depalletizer. The empty crates pass through the unscrewing machine, and the glass bottles are unpacked by the decrating machine onto the container conveyor. The bottles are transported to the bottle cleaning machine, where they are cleaned and disinfected. The bottles are inspected for damage and remaining impurities by the empty bottle inspector and are then filled and capped with product in the filling and closing machine. The filled bottles are inspected in the full bottle inspection machine for, e.g., glass splinters, and labels are applied in the labeling machine. The bottles are then packed in previously cleaned crates in the crating machine and stacked on pallets by the palletizer. The crate bypass stream is represented in simplified form by a crate magazine, since a complex throughput system for the crate transport is implemented in the real plant. In the pallet stream, the pallets are also buffered in a magazine.

In addition, a returnable PET beverage bottling plant is used as part of a use case. The plant follows the scheme shown above but differs in the additional machines and in the design of some machines. For example, a sniffer which detects the previous product of a bottle and rejects the unwanted bottles accordingly is used. In addition, a rinser and a flash pasteurizer are in operation. The filling process is further described in detail, among others, by Manger [50].

Both plants are connected to an in-house data acquisition system (DAQ). The mode, operating status, and electrical energy consumption of each individual unit (see Figure 3) are recorded every two seconds. In addition, the demand for thermal energy, water, CO_2, and compressed air is recorded for the entire plant. The data points follow the declaration of the Weihenstephan Standards [51], which are a standardized data interface between the individual machines and a higher-level system. It defines the unique and standardized semantics of the individual data points as well as the transmission method. This makes it possible to receive and process equivalent data from each machine, regardless of the manufacturer.

The database of the returnable glass bottling plant comprises two measurement campaigns, the first covering a period of two months and the above-mentioned data scope. In contrast to the period of the second measurement campaign, the first data collection was characterized by an almost continuous production (apart from the weekend). For external reasons, the beverage bottling plant was in operation for only about 3 days per week during the second period (4 weeks). The individual units were equipped with measuring devices for recording the demand for compressed air and were connected to the DAQ. Further, units such as the empty bottle inspector, the full bottle inspector, and the decorker were added to the current measurement. The only consumer of thermal energy and water is the bottle cleaning machine, as its warm wastewater is used for the crate washer. The filling machine is the only unit requiring CO_2 for the production of certain articles. A manufacturing execution system (MES) served as a source, for both plants, for detailed plans, which includes the production times, quantities of the articles produced, and long downtimes, caused by failures as well as maintenance and cleaning. The database for the returnable PET bottling plant comprises a period of 2 months, including data points such as the mode, the operating state, as well as the electrical energy demand of all machines.

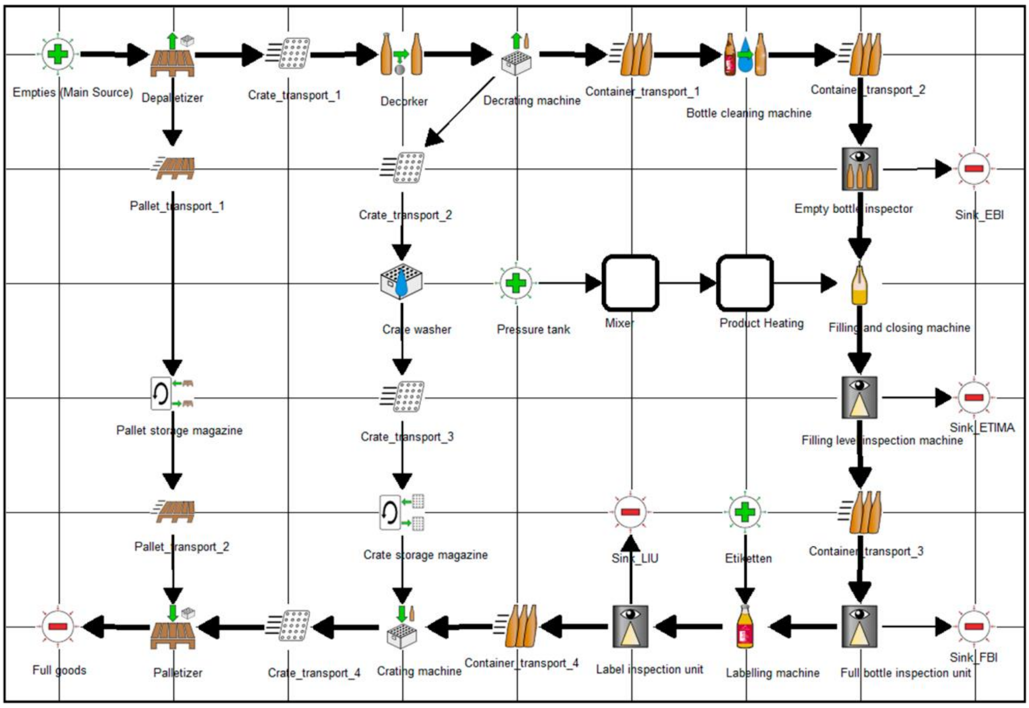


Figure 3. Layout and units of the simulated beverage bottling plant in the modeling editor (detailed version as presented by Bär et al. [48]).

The measured data from the DAQ are converted to a uniform data structure, which also serves as the structure for the data generated by the simulation. The data within the structure are divided into interval data, which include information such as the mode and operating state, and timestamp data, which cover all data, such as consumption values. The corresponding machines as well as data points are referenced via keys, which allows for an easy extension of the data structure.

3. Energy Consumption Behavior

Based on the findings of Osterroth et al. [36], the operating state-related consumption behavior of packaging machines is used in the modeling and simulation and assigned to the following energy and media types: electrical energy, thermal energy, compressed air, water, and CO_2. The time-dependent intermediate-level application is omitted due to the granularity of the modeling on the unit level (see Chapter 5). In the definition of the consumption levels, the operating mode (WS_Cur_Mode) and the operating state (WS_Cur_State) [51], which is described by a state model, are used. Table 1 shows the assignment of the individual modes and states, which appear in the real data, to the consumption levels.

O_L is described by the off-mode (inactive) in the data point WS_Cur_Mode. This is present in standstill, e.g., on a weekend in which no production is planned. It is proven that most of the units also have a demand for energy and media in this case [36]. During production, the listed operating states (WS_Cur_State) can be present. These are basically divided into the normal operation of the machine (C_L), a lack or tailback situation (D_{L1}), as well as failure situations (D_{L2}).

Table 1. Assignment of the consumption levels according to WS_Cur_State/Mode (Mode/State and Integer coding).

Consumption Level	Description	Value of WS_Cur_State	Value of WS_Cur_Mode
O_L	Off-level (Inactive)	-	Off (1)
D_{L1}	Downlevel in Lack/Tailback	Prepared (04) Lack (08) Tailback (16) Lack_Branchline (32) Tailback_Branchline (64)	Automatic (4)
C_L	Consumption Level in Operating	Operating (128) Idle (32768)	
D_{L2}	Downlevel in Failure	Equipment_Failure (1024) External_Failure (2048) Emergency_Stop (4096) Held (16384)	

4. Determination of Simulation-Relevant Parameters

For an automatic determination of simulation parameters, such as consumption levels as well as parameters for the description of the failure behavior, an evaluation software was developed. The parameters can be specific to various evaluation criteria, such as article-based, container type-based, or based on any time periods.

The mean consumption levels of the individual energy and media types are calculated in the intervals in which the same operating state is present. In addition to the machine-specific determination of the total consumptions, a detailed statistical evaluation of the consumption values (weighted mean value, standard deviation, variance, standard error, and 95% confidence interval) is performed.

Failure behavior is determined using the operating state of a machine [22]. The TTR (Time To Repair) refers to the duration of downtime, while the downtime-free running time between two successive downtimes is defined as TBF (Time Between Failures). To determine the TTR, the times of the states of the D_{L2} are combined, and for the TBF, the states of the D_{L1} as well as C_L are combined (see Table 1). The availability results are shown in Formula (1).

$$\text{Availability} = \text{MTBF}/(\text{MTBF} + \text{MTTR}) \tag{1}$$

In addition, the operating and downtimes are examined with regard to the distribution curve of the failure behavior. The suitability of the Weibull, negative exponential, and lognormal distributions was examined by Voigt [22], whereby the Weibull and exponential distribution achieve the best fit. This could be confirmed graphically by means of histograms and QQ-plots, including the chi-square test. The neg. exponential distribution is used in this work because random failures with a constant failure rate are assumed, and this describes the behavior sufficiently accurately. Moreover, the exponential distribution can only be described by one variable (β) [22].

Apart from the data from the DAQ, it is necessary to determine further parameters directly in the plant. Therefore, the topological data of the plants as well as all machines and transport equipment were determined as part of performance analyses in accordance with DIN 8743 [52]. The set performance of all individual units was analyzed using measuring light barriers and manually by means of a minimum triple determination. Further, the capacities per filling article of the individual units as well as the global rejection rates of inspection machines were determined. All buffer sections were investigated with regard to their buffer capacities and times.

5. Modeling Approach

Since modeling is one of the biggest barriers for SMEs, a modeling editor, presented by Bär et al. [48], was used. The editor was developed with special attention to a user-friendly and simple application to enable modeling for users without a specific pre-qualification. This was successfully validated and demonstrated by using a systematic test and exemplary simulation studies. The holistic modeling of production systems with respect to their energy and media consumption is made possible by the use of context-free modeling columns. The editor generates a standardized XML-based configuration file, which contains all required simulation-relevant parameters and structures of the columns, for any subsequent simulation environment. The parameters must be entered manually in the modeling editor. Numerous help functions support the user, and the modeling can be simplified and accelerated. The modeling approach implements existing standardizations, such as ANSI/ISA S88 [53]. The modeling columns consist of a physical model to represent real existing plants, a process model to represent batch production processes by an article model and a production plan model. The modeling depth of the editor is to the unit level (e.g., the filling machine). This is mainly related to the scope of the required parameters as well as to the complexity and accuracy of the models and is sufficiently discussed by Bär et al. [48]. If the batch-oriented production process is modeled, the process model, which describes the energy and media consumption behavior at the process operation level, is used. The article model allows for the modeling of different filling articles, which can be produced on the process cells of the physical model. Each unit can be parameterized with regard to its consumption and performance-describing parameters, but also with regard to the container type, as well as the packaging ratios. The production plan model describes the production to be processed in the simulation. It comprises, inter alia, a shift plan for the definition of the production and non-production times [52], e.g., a weekend, when no production is planned. Further, a sequence plan, which determines the sequence of the articles and quantities to be produced, is defined. In a matrix table, the required changeover and cleaning times, which are required between the articles in the sequence model, are determined.

6. Simulation Environment

All simulation studies were carried out using the “PacSi” simulation environment [54] developed by SimPlan AG, Dresden, Germany. The software follows a discrete-time approach with regard to the applied simulation method and is based on a simulation of the material flow. The simulation environment is further described by Römisch and Weiß [55] and was used for various applications [21,56]. Model creation within the software is based on building blocks, which differ fundamentally in functionality, the separation and merging of material flows, and parameter sets. The individual units are assigned a stochastic failure behavior, and failure propagation is achieved by the chaining of the machines by transport devices.

Failure behavior is described by the variation, by means of a random number generator, of the seed key, which initializes a random number stream. Thus, these streams for the MTTR and MTBF are newly generated according to the distribution function (negative exponential) with each simulation run, and the times and durations of the failures are varied. Therefore, different results are obtained with each simulation run, whereby statistical certainty can be achieved over long simulation durations, on the one hand, and multiple repetitions of the experiments, on the other.

In the scope of this work, the simulation environment was extended by numerous functions. The most important extension is the automatic generation of simulation models based on the configuration file of the modeling editor. The different specific building blocks of the modeling editor are therefore mapped to the existing ones of the simulation environment. By using a coordinate system as well as the edges of the elements in the modeling editor, the topology and logical structure can be reformulated in the simulation environment. During simulation model creation, the parameter sets of all units are loaded from the configuration file and reformulated if necessary, and the simulation model is parameterized. A special feature here is the integration of a production plan, i.e., the shift plan, the sequence of different recipes and articles, as well as the changeover matrix. This is mainly solved by sources, elements in which material is released in the simulation, by storing the non-production times as well as the times between the recipes/articles and their specific article number. This indexing allows for an element-specific parameter change and thus enables a recipe/article-specific simulation within the production plan. Non-production times defined by the shift model are also a special feature, as the newly implemented off-consumption level (O_L) is active in this time. Consumption in the production times is described by the respective operating state. The simulation results, which are generated every second, are stored in a SQLite database.

7. Evaluation, Verification, and Validation

The aim of verification and validation is to reduce the erroneous statements of simulation studies and thus to minimize the risk of the resulting wrong decisions. Verification involves the transformation of a model from one type of representation to another. In the present case, the correct transformation of the model from the modeling editor to a simulation model is meant. Validation, in turn, is to ensure the correct behavior of the model in relation to the original model. The validity of the model for the specific application purpose is checked [42].

For validation, the corresponding periods were simulated with 10 repetitions. The simulation results of the cumulative consumption of the entire plant and the individual units were each statistically examined. The mean values were compared with the corresponding real values, and the percentage deviations were calculated. Furthermore, the consumption values with regard to the individual filling orders were determined and compared with the real values. The production counter of the filling machine constitutes the reference point for the end or start of a filling order. In parallel, the production quantities and times were determined and compared with the real values. Use cases should, among other things, reveal the optimization potential with regard to the energy and media efficiency of the beverage bottling plants investigated in the validation periods presented. The savings achieved should be higher than the deviations determined in the validation to avoid erroneous statements.

8. Results

8.1. Validation Periods and Parameter Determination

Two different time periods considering different factors are available for validation. Validation period 1 comprises the electrical energy demand of the units, and an extensive production schedule including non-production times such as a weekend is simulated. Validation period 2 includes the full energy and media demand of the units of the beverage bottling plant, but a shorter time period with only two articles is included.

Consumption parameters were article-specifically determined for period 1 and container-type specifically for period 2, due to the insufficient article-specific database here. According to Sargent [57], the orders of the articles produced within the validation periods were not included in the periods of consumption parameter determination. The values describing the failure behavior of the machines were determined specifically for the corresponding orders in the validation periods. A detailed overview of the validation periods with regard to the articles produced as well as the production times and quantities is given in Table 2.

Table 2. Validation periods including produced articles (quantities and times) as well as the extent of the consumption parameter determination.

Validation Period	Article	Article Information	Output (Bottles)	Duration [h]	Changeover Time (to Next Article) [min]	Extent of Consumption Parameter Determination [h]
1; (193.2 h)	1	Mineral water sparkling; 12 × 0.5 L	417,521	21.8	46	19.60
	2	Mineral water low sparkling; 12 × 0.5 L	425,552	20.4	99	35.72
	3	Mineral water still, 12 × 0.5 L	377,060	19.7	252	18.97
	4	Mineral water still, 12 × 0.75 L	1,339,097	79.2	-	347.81
2; (61.9 h)	4	Mineral water still, 12 × 0.75 L	1,248,702	59.0	80	380.83
	5	Lemonade 12 × 0.75 L	35,285	1.7	-	

The real data recorded by the DAQ of the production plan were converted to the presented data structure, and the simulation-relevant parameters were determined automatically by executing a self-programmed software in MATLAB 2020b. This resulted in a total of approximately 1250 parameters for all five articles. Table A1 (Appendix A) shows the state-related energy and media-specific mean consumption data for each consumption level, including the 95% confidence interval, and the failure behavior data (within the validation period) exemplary for article 4. The correct operating status reports of the individual units were randomly checked during operation. The changeover times between the individual articles for possible required conversions or cleaning were taken from the validation periods of the real data. The basis for this is the production counter of the filling machine (no increment over a longer period means a changeover). Due to the lack of repetitions, it was not possible to consider several changeover periods.

8.2. Model of a Beverage Bottling Plant

The beverage bottling plant investigated in this work was modeled in the described editor (Figure 3) and is a more detailed version, as already presented by Bär et al. [48]. The main differences are due to the representation of further units, such as inspection machines, decorker, etc., which could be examined within the scope of the additional data acquisition. The main material flow (thick arrows) starts with the main source at the top left and runs clockwise to the source at the bottom left. The two secondary flows (thin arrows) for pallets and crates are located on the left side and in the middle, respectively. The articles produced in the validation periods were modeled with article-specific parameters in each case.

The present model covers a much larger scope than already presented, since numerous articles, including their article- or container-specific parameters, are modeled. In addition, the schedule within the production plan was parameterized with the articles and production quantities per filling order listed in Table 2. The changeover times were transferred to the matrix to define the times between the individual articles. The shift times for validation period 1 could be determined from the real data (non-production from Saturday 08:30 am to Monday 07:00 am) and were parameterized in the modeling editor.

8.3. Verification and Validation

8.3.1. Model and Simulation Verification

A verification of the model creation and the function of the simulation environment was performed by hand in three steps. Therefore, the configuration file from the modeling editor was loaded in the simulation environment, and the model was generated automatically. The topology of the beverage bottling plant and the correct connection of the elements were successfully checked. After a simulation run is started, the respective unit- and article-specific parameters are loaded. By regularly stopping the simulation to check all articles, the parameters were successfully compared with those of the model in the modeling editor. A verification of the correct functioning of the simulation environment was performed using the result data, which were analyzed, on the one hand, using the open source software HeidiSQL_11, which allows access to, and the viewing of the SQLite databases; and, on the other hand, via the described evaluation tool. In particular, the application of the correct consumption levels with regard to the operating status of the individual unit was checked. In addition, the main source, which is the origin of the main flow and thus represents the production plan, was checked for correct functioning with regard to production quantities and changeover times. In all cases, the verification was carried out continuously with the development process of the simulation environment and was successfully completed.

8.3.2. Validation of Energy and Media Demand in Period 1

The focus in the first period is on electrical energy consumption and on the complex production plan. Figure 4 shows the measured and simulated electrical energy consumption of the beverage bottling plant. The subdivision shows the four articles, which differ by a distinct total power requirement, as well as the production-free weekend, which represents idle time (duration 46.25 h) [52].

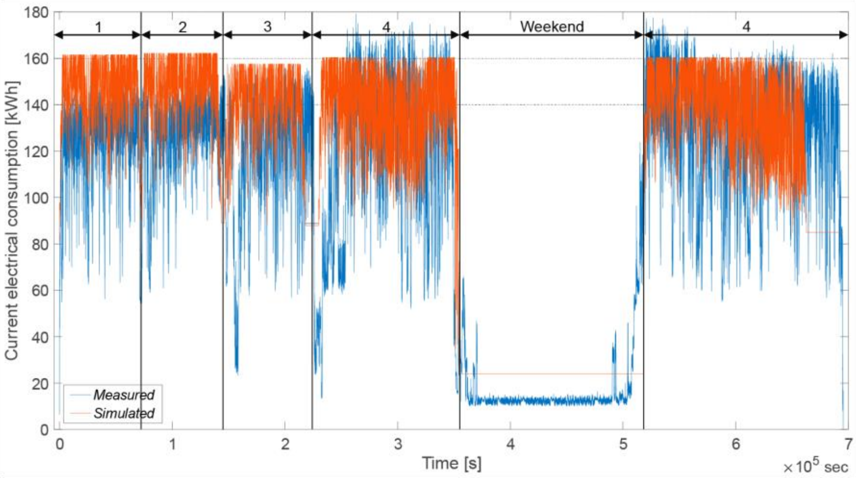


Figure 4. Total current electrical consumption in kW (blue: measured values; red: simulated values) of the beverage bottling plant in validation period 1 (193.2 h); Subdivision in articles (1–4) as well as a weekend (idle time).

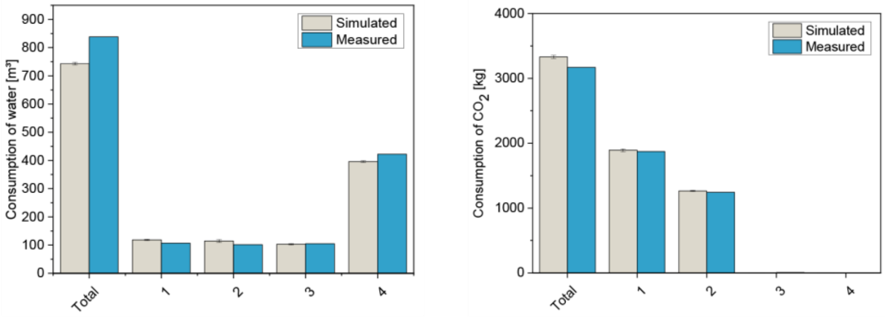
The production quantities of all articles show a deviation of less than ±0.1% compared to the real production counter of the filling machine. The production times of article 1 and 2 are within a range of approx. −6–8% compared to the determined real-time periods. Article 3 shows a deviation of approx. −4.5%. Article 4 shows a total deviation of −11.2%, i.e., an accelerated production within the simulation.

Table 3 shows the mean values of the simulated data and the percentage deviation of these data from the real data for the entire period, as well as the individual production periods of the articles. Starting with the entire plant, the individual units are listed in descending order of their electrical energy demand. No measured data are available for the decorker, empty bottle inspector, and full bottle inspector, as these could only be included in validation period 2. The bottle cleaning machine, the crate conveyors, and the mixer could be clearly identified as the main consumers of electrical energy. These account for about 70% of the total amount of electrical energy and consistently show a very small percentage of deviation from the measured data. The bottom 50% of the units account for only 12.3% of the total amount of electrical energy. Over the entire period, a percentage deviation of 0.33% for the electrical energy demand of the entire plant could be determined. In the article-specific validation, it is noticeable that units such as the filling machine, the pallet transport, and the depalletizer show quite high deviations. The large deviations at article 4 are due to a long downtime (lack of staff in the plant and in the supply) at the beginning of the article, which can be explained by the malfunction reports. Since long downtimes only occur very rarely due to the failure behavior distribution, the simulated production runs faster and reaches the planned production quantity earlier.

Table 3. Consumption of electrical energy in kWh (measured value (Measured), mean simulated value (M), 95% confidence interval (95% CI), percentage deviation between measured and simulated (PD [%])) in validation period 1 as well as the article production periods.

Machine	Total Validation Period 1				Article 1	Article 2	Article 3	Article 4
	[kWh]	Simulated						
	Measured	M	95% CI	PD [%]	PD [%]	PD [%]	PD [%]	PD [%]
Total	20,282.1	20,349.8	26.67	0.33	−4.83	−5.3	−5.45	−8.42
Bottle cleaning machine	7070.0	7060.9	5.64	−0.13	−9.45	−7.07	−8.06	−7.69
Crate transport	3686.0	3690.9	26.94	0.13	8.31	2.32	−3.72	−15.79
Mixer	2967.0	3171.5	0.46	6.89	−2.8	−8.97	4.72	−5.18
Container transport	1437.8	1471.6	5.59	2.35	4.73	8.89	8.39	5.24
Filling machine	1450.0	1342.0	0.71	−7.45	−23.53	−8.54	−23.97	−9.84
Crate washer	1216.2	1186.2	0.86	−2.47	−10.04	−20.26	−8.56	−6.48
Labelling machine	510.9	537.2	0.22	5.14	−9.42	−9.15	−2.34	−0.82
Decorker	-	498.6	0.26	–	-	-	-	-
Pallet transport	473.0	473.8	1.19	0.17	36.48	30.29	−19.76	−26
Palletizer	440.8	423.9	0.31	−3.83	−6.76	−3.9	−8.44	−12.24
Depalletizer	407.1	370.4	0.04	−9.03	−12.35	−30.4	−16.47	−17.33
Crating machine	315.7	315.3	0.33	−0.14	−8.57	−8.55	14.72	−6.03
Decrating machine	307.6	306.3	0.09	−0.43	−9.09	−8.28	−6.91	−5.86
Empty bottle inspector	-	148.1	0.00	-	-	-	-	-
Full bottle inspector	-	85.3	0.01	-	-	-	-	-

Figure 5 shows the consumptions of water and CO_2 within validation period 1. Since articles 3 and 4 are “mineral water still”, no CO_2 is required. The total consumption shows a deviation of approximately 5% compared to the measured value. The water consumption of the bottle cleaning machine shows an overall deviation of −11%.



(**a**) (**b**)

Figure 5. Comparison of the consumption of water [m^3] (**a**) and CO_2 [kg] (**b**) in validation period 1 (measured value, mean simulated value, 95% confidence interval) as well as the four production article periods.

8.3.3. Validation of Energy and Media Demand in Period 2

Validation period 2 is primarily used to validate the compressed air and thermal energy consumption. The parameters determined were also used in validation period 1. The production quantities of both articles (4 & 5) show a deviation of less than ±0.1%

compared to the real production counter. The production times of articles 4 and 5 show a small deviation of approx. −3 to −3.5% compared to the production times required in reality. Figure 6 shows the current electrical energy demand and Figure 7 the current demand for compressed air of the bottling plant (measured versus simulated). In each figure, a downtime (approximately 5 h) due to a technical defect can be seen at the beginning as well as at the end. During the remaining production period of article 4, the output of the filling machine was increased, while the filling machine in the simulation runs with the parameterized set performance. The changeover to article 5 (production time 1.7 h) can be seen toward the end of the simulation.

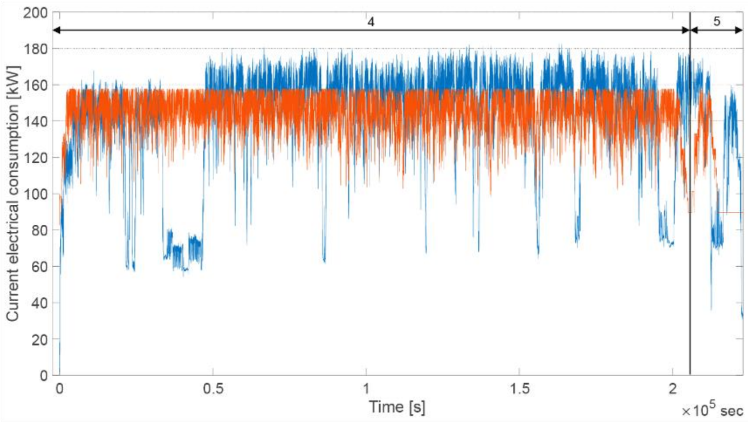


Figure 6. Total current electrical consumption in kW (blue: measured values; red: simulated values) of the beverage bottling plant in validation period 2 (61.9 h); Subdivision in articles (4 & 5).

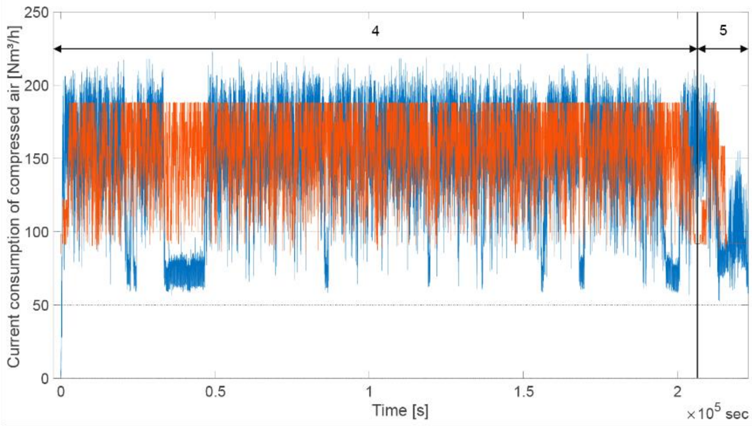


Figure 7. Total consumption of compressed air in Nm^3/h (blue: measured values; red: simulated values) of the beverage bottling plant in validation period 2 (61.9 h); Subdivision in articles (4 & 5).

Table 4 shows the electrical energy consumption in validation period 2. An overall good fit with a percentage deviation of 0.14% is achieved, as the largest consumers show a small deviation (about ±3%). Units such as the depalletizer and palletizer, together with the container transport, show the largest deviations. The deviations (electrical energy and compressed air) of the time period of article 4 correspond to the values of the entire period. The deviations for article 5 are noticeably higher, as the article covers only 2.7% of the total time and is therefore strongly affected by the delimitation method of the articles.

Table 4. Electrical energy consumption in kWh (measured value, mean simulated value (n = 10), 95% confidence interval (95% CI), percentage deviation between measured and simulated) of the validation period 2 as well as the article production periods.

Machine	Total Validation Period 2				Article 4	Article 5
	[kWh]	Simulated				
	Measured	M	95% CI	PD [%]	PD [%]	PD [%]
Total	8766.5	8779.1	10.15	0.14	0.42	13.54
Bottle cleaning machine	3052.4	2958.4	3.89	−3.08	−6.04	5.01
Mixer	1459.2	1517.3	0.00	3.98	−0.69	28.61
Crate transport	1524.1	1493.0	6.63	−2.04	−5.64	15.74
Crate washer	490.7	538.1	0.11	9.68	5.68	34.02
Container transport	467.7	530.2	2.41	13.38	10.00	9.20
Filling machine	527.6	504.7	0.12	−4.33	−6.83	0.69
Labelling machine	221.1	233.1	0.12	5.45	1.50	9.49
Decorker	190.4	183.5	0.21	−3.63	−3.14	−2.86
Palletizer	179.7	162.4	0.12	−9.60	−12.40	53.08
Pallet transport	149.0	159.9	0.67	7.31	7.31	−16.03
Depalletizer	164.9	149.2	0.05	−9.57	−12.19	5.22
Crating machine	117.6	120.6	0.20	2.58	−3.22	8.97
Decrating machine	111.5	115.6	0.07	3.64	0.03	30.05
Empty bottle inspector	53.0	51.9	0.02	−2.09	−4.29	2.83
Product heating	29.5	32.5	0.00	9.86	14.30	11.50
Full bottle inspector	28.3	28.7	0.00	1.60	−2.32	−29.63

Table 5 shows the consumption of compressed air for validation period 2. The four largest consumers account for about 70% of the total compressed air demand. The small deviations between the simulated and measured data of these units result in a small overall deviation. For units such as the decorker and the cycle-based depalletizers and palletizers, there are large deviations. Due to the small share of the consumption of the product heating, the high deviations are not decisive to a good agreement of the total consumption.

Table 5. Consumption of compressed air [Nm^3] (measured value, mean simulated value (n = 10), 95% confidence interval (95% CI), percentage deviation between measured and simulated) of the validation period 2 as well as the article production periods.

Machine	Total Validation Period 2				Article 4	Article 5
	[Nm^3]	Simulated				
	Measured	M	95% CI	PD [%]	PD [%]	PD [%]
Total	9348.3	9354.3	8.39	0.06	−1.26	8.22
Labelling machine	1962.7	2006.5	1.02	2.23	−1.62	−4.76
Crating machine	1740.1	1665.4	4.20	−4.29	−9.53	54.95
Filling machine	1548.0	1546.7	0.08	−0.08	−2.69	6.23
Empty bottle inspector	1162.6	1179.2	0.03	1.43	−1.09	9.50
Decorker	573.4	703.8	5.36	22.74	−5.03	−17.87
Full bottle inspector	562.7	568.7	0.00	1.07	−2.16	1.50
Decrating machine	575.8	555.5	0.14	−3.52	−11.95	6.93
Palletizer	475.3	415.4	0.49	−12.62	−14.80	51.23
Depalletizer	369.3	319.9	0.26	−13.38	−15.37	−11.48
Bottle cleaning machine	318.2	314.0	0.24	−1.35	−5.11	10.32
Product heating	35.1	43.3	0.00	23.36	20.76	7.53
Mixer	30.5	31.0	0.00	1.71	2.41	27.07
Crate washer	5.3	5.0	0.00	−7.43	−10.96	31.19

A comparison of the CO_2 consumption values is not useful, as CO_2 is needed only for article 5. The values of the thermal energy demand deviate by a total of +13.61% and the values of the water consumption by +6.14%. These occasionally large deviations are due to the relatively short validation period.

8.4. Application of the Method in Use Cases

In one use case, the replacement of the main consumer, the bottle cleaning machine (year of construction 2012), was analyzed. During parameter determination, it was ascertained that the consumption values for thermal energy and water significantly exceed the values during the warranty acceptance test after the completion of the plant. Water demand was determined to be 284 mL/bottle (originally 140 mL/bottle) and the thermal energy demand 15.5 Wh/bottle (originally 9.5 Wh/bottle). In addition, the availability of the bottle cleaning machine has noticeably decreased, from 90% to 86%. The background to the changes is unclear. To be able to examine the effects on the overall system in validation period 2, the consumption levels of the individual operating states and performance values were adjusted according to the original values. These values agree with the currently common values determined by Osterroth et al. [20], as well as with the authors' own empirical values. The adjusted model was simulated with a tenfold repetition and compared with the total values of the validation. As shown in Table 6, enormous savings of thermal energy and water demand were determined. Since the bottle washer is the sole consumer of these types of energy and media, there is a direct connection. The demand for electrical energy of the entire system is also influenced. The water savings alone correspond to a cost saving per year in the mid five-digit range (at an average water price of 2 € per m^3 and a production time of 5 days for 50 weeks a year). Added to this are the sustainable aspects of reduced wastewater production and the required purification of the water.

Table 6. Consumption values and savings of the thermal, electrical, and water demand of the beverage bottling plant before and after the adjustment of the consumption values of the bottle cleaning machine.

Simulation Run	Time [h]	Consumption of		
		Thermal Energy [kJ*10^3]	Water [m^3]	Electrical Energy [kWh]
Original	61.9	68,100	347	8600
Adjusted	58.7	40,452	175	8284
Savings [%]	5.1	40.6	49.6	3.67

In a further simulation study, the suitability of the method is shown with regard to the simulation of multiple beverage bottling plants. For this purpose, the returnable glass and the PET bottling plant were modeled with specific articles and production plans over a period of 8 days. The load profile for, e.g., electrical energy can be determined by the simultaneous simulation of both plants. This information can be of considerable interest in the design of supply facilities, such as the electricity supply, for example, in order to be able to make an efficient and cost-effective investment. Figure 8 shows the operation of the two beverage filling plants and their total electric energy consumption in validation period 1 (including a weekend as an off-period).

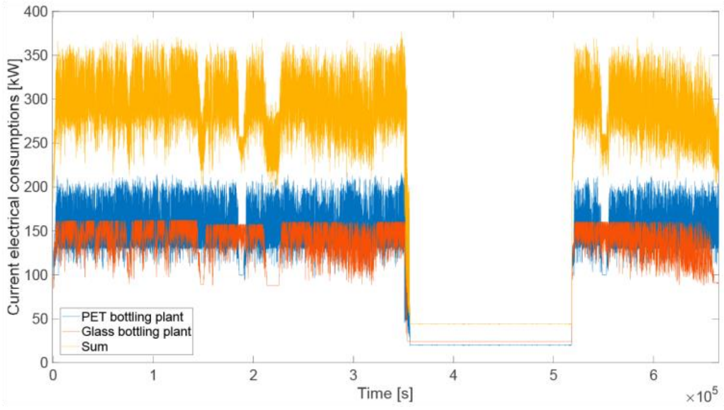


Figure 8. Current electrical energy consumption of the bottling plants and their total in kW.

9. Discussion

The simulation-relevant parameters were determined using the presented evaluation method. Due to the extensive database, the article- and container-type-specific parameters could be defined. Overall, they show very small confidence intervals (see Table A1).

The use of the described data structure could be an opportunity for SMEs and machine manufactures. If data are available in this format, the evaluation tool enabling a fast, easy, and flexible determination of simulation parameters as well as the evaluation of simulation experiments can be used. This can sustainably overcome the barriers for modeling and encourage SMEs to expand their data collection. The modeling editor proved to be a good support by modeling the plant as well as all articles and the production plan in a structured and standardized way via modeling columns. Thus, errors in simulation model generation can be avoided.

For the first time, a simulation environment incorporates a detailed production plan including non-production times and an associated off-consumption level. In addition, articles can be simulated with specific parameter sets, and the times required for changeovers can be specified. The automated simulation model generation based on the configuration file could be demonstrated and successfully verified in the example of a simulation environment. Since it contains all simulation-relevant parameters and information and is clearly structured, this could also be implemented in other simulation environments. The combination of the modeling editor and the simulation environment opens up a great flexibility with regard to the mapping of production systems and has already been demonstrated [48]. Compared to a time-consuming manual parameter determination and simulation model creation, which can take several days, depending on its complexity, the present models could be created within a few hours using the modeling editor, and an executable simulation model including all aspects could be generated. However, this requires the availability of data according to the presented data structure. A fast model generation represents a decisive advantage for companies of any size.

Based on two production periods of a beverage bottling plant, the extensive validation is intended to underpin the suitability of the entire method with regard to several factors. A comparison of the measured and simulated values was conducted. The focus in the first validation period is primarily on the production schedule with different articles and non-production times as well as the electrical energy consumption. The production quantities determined in the simulation match those of reality.

An explicit validation of the off-periods (e.g., the weekend in validation period 1) does not take place. The graphical comparison (see Figure 4) illustrates a similar consumption in this period, but could be improved. The deviations in the electrical energy demand of the entire plant in the first validation period are very low and are achieved by the good fit of the main consumers. Machines such as the de-/palletizer and the mixer show the largest deviations. This reflects the findings of Osterroth et al. [36], as the operating state-related consumption behavior does not fit perfectly for these units. No adjustment was made due to suitability for the remaining units.

The accelerated production in the simulation has two causes. On the one hand, the start-up times of the plant in the event of a changeover cannot be represented well enough in the simulation. In particular, the individual changeover work on individual units must be mentioned here, as the changeover time is related only to the filling machine. During flying changeovers, various articles are usually active on the plant. This explains the greater deviations of the article-specific consumptions. A more precise assessment is possible only if each machine provides information on the subject of articles as well as on the current program. In addition, it is not possible to model or simulate any lower outputs of the units in the start-up and shutdown phases. On the other hand, due to the neg. exponential failure behavior, long failure times occur only rarely in the simulation and are difficult to reproduce. Together with all the delays that occurred during real changeovers, this situation corresponds approximately to the time difference between the measured and the simulated total time. The long downtimes that occurred in real production must be documented to make deviations comprehensible.

The deviations in CO_2 demand are within acceptable limits, and a consumption behavior related to the operating condition can be confirmed. Water demand deviates strongly for article 2, which in turn strongly influences the overall deviation. This can be explained due to the cyclical filling of the baths of the bottle cleaning machine. However, the deviation of article 4, which has the largest database, is in an acceptable range of about −6%.

Validation period 2 includes the simulation of all energy and media types, but for a shorter period. Here, too, the deviations in production times can be traced through fault logs. The deviations in the required electrical energy quantities mirror the findings of period 1. Due to the extensive database, an overall very low deviation is achieved, especially for compressed air. Here, the consumption parameters were determined in relation to the container type. For the depalletizer, palletizer, and decorker, very high deviations were found and the operating-condition-related consumption behavior can be doubted, due to the low confidence intervals of the parameters. The deviations in the thermal energy demand of the bottle washer are relatively high and can be attributed to the short period as well as to the cyclical heating of the caustic and should continue to be investigated more deeply.

One use case investigates a theoretical reduction in energy and media demand. Modernizing the bottle cleaning machine achieves savings significantly higher than the deviations in the total values within validation period 2. A second use case shows the simulation results of two different beverage bottling plants to illustrate the breadth of application of the method. The simulation studies underpin the suitability of the overall method. Nevertheless, human intelligence is needed to evaluate the simulation results and decide on the next steps that will ultimately affect system efficiency [58].

In comparison with Osterroth et al. [36], the operating-state-related consideration of consumption without the application of time-dependent intermediate levels provides a similar or a sufficient accuracy of the validation results. Particularly when considering complex overall systems, the simplified application facilitates the creation of the model, and the consideration at unit level satisfies the requirements.

10. Conclusions

To perform quick and easy forecasts of the energy and media demand of holistic beverage bottling plants, especially for SMEs, an approach for modeling and automatic simulation model generation was presented. This can be a chance for SMEs to reach a more sustainable production. This is made possible by a modeling approach implemented in a user-friendly editor. In combination with a standardized data format and evaluation software, simulation-relevant parameters such as consumption and failure behavior data can be determined automatically. The prerequisite for this, however, is a sufficiently large database. The approach was applied to a beverage bottling plant and a model with various articles, and, for the first time, a detailed production plan was modeled. Based on an XML-based configuration file, the simulation model was automatically generated. This represents an enormous time saving compared to manual model creation.

The detailed validation of the entire method by comparing the simulated consumption values of two different time periods to the measured values shows that the approach is well suited to provide reliable forecasts. The respective main consumers of the energy and media types are decisive, which confirms the granularity chosen in the modeling environment. This is also underpinned by Hubert [39]. Therefore, units such as the depalletizer, palletizer, mixer, and decorker, which sometimes show strong deviations compared to the measured values, can be mostly neglected depending on their share in the total consumption. For the first time, a detailed, machine-related compressed air consumption was determined and analyzed. The compressed air consumption, as well as the consumption of water and CO_2, follow the consumption behavior presented. Furthermore, the validation of the thermal energy demand does not show a good fit, which means that the consumption behavior approach should be expanded. Further deviations in the validation can be explained with the help of fault logs. A recording of the current program of the machines as well as the extension for mapping start-up/shut-down ramps and the improvement of changeovers in the simulation environment would further increase the accuracy. Simulation studies support the validation of the method, in which savings exceeding the deviations of the validation results could be achieved. One challenge is the epistemic uncertainty, i.e., the lack of knowledge on how to interpret the results and how to design further steps, e.g., simulation experiments, and also the imprecise and coarsedata and information for the modeling and parameterization of simulation models. Decision models can help here [59].

The method proved to be suitable for creating models of complex bottling plants and automatically generating simulation models. In the future, it is intended that SMEs will only use the presented modeling editor [48] to apply the method. Starting from this, the model of the production system to be simulated is automatically passed on to a cloud-based simulation environment, where the simulation is performed, and the results of the simulation are reported back. The only points of contact are the modeling editor and the output data, which can be processed, e.g., with the help of the evaluation tool, and a deeper knowledge of XML and the simulation method will not be required. If, in addition, the production data is available in the presented data structure, the barrier of the data basis is overcome, and the simulation parameters can be determined automatically. The overall solution is intended to reduce the personnel and cost effort, and thus enable SMEs to test optimization strategies and make possible sound investment decisions. The approach provides an opportunity to improve energy efficiency and, as a result, product efficiency. To extend the approach and to include, in this case, the material efficiency, the next logical step is the mapping and simulation of a holistic production plant, such as a brewery. A challenge here is the mapping of the batch-oriented operation of the process area and the associated different energy consumption behaviors. A combination of both areas would, for example, allow for the investigation of recuperative energy use as well as overall consumption profiles. This represents an opportunity to save energy and media and to reduce raw materials and waste accordingly, and is a step toward sustainable production.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. Parameters for article 4; ([1] container-specific parameter determination from the second measurement period; [2] specific parameters for transport equipment: length, transport speed, capacity; [3] determined in the validation period).

Unit	Set Performance [b/h]	Capacity [bt]	MTBF [s] [3]	MTTR [s] [3]	Availability [%]	Electric Consumption [kW]								Compressed Air Consumption [Nm^3/h] [1]							
						C_L		D_{L1}		D_{L2}		O_L		C_L		D_{L1}		D_{L2}		O_L	
						MW	95% KI	MW	95% KI	MW	95% KI	MW	95% KI	MW	95% KI	MW	95% KI	MW	95% KI	MW	95% KI
Depalletizer	40,039	108	396	44	89.9	3.36	0.012	1.38	0.012	1.41	0.025	1.13	0.04	7.99	0.024	1.98	0.025	3.25	0.053	0.12	0.062
Decorker [1]	32,280	12	600	12	98.0	3.65	0.051	3.3	0.024	3.3	0.033	0	0	24.82	0.056	24.82	0.016	0.52	0.021	0	0
Decrating machine	31,147	96	821	34	96.0	2.13	0.006	1.39	0.006	0.97	0.019	0.9	0.019	12.73	0.026	1.52	0.019	0.7	0.116	0.27	0.167
Bottle cleaning machine	30,640	9425	471	104	81.9	50.42	0.058	40.03	0.11	40.4	0.21	2.00	2.33	4.91	0.012	5.51	0.053	5.59	0.042	4.34	0.794
			Thermal energy consumption [kW]			33,403	2706	2227	4507	282.05	5.353	20.69	13.419								
			Water consumption [m^3/h]			7.52	002	0.01	0004	0.03	0.006	0	0								
Empty bottle inspector [1]	28,998	1	433	68	86.4	0.93	0.005	0.61	0.006	0.61	0.009	0.64	0.075	20.73	0.022	14.84	0.025	14.59	0.038	14.18	0.271
Filling and Closing machine		120				8.95	0.021	6.28	0.02	5.97	0.045	3.72	0.221	26.96	0.04	20.12	0.089	19.93	0.137	7.03	0.6
			CO_2 consumption [kg/h] (article 1)			10,628	1765	6273	4378	60.97	4.599	1.37	1.692								
Full bottle inspector [1]	33,197	1	2465	18	99.3	0.49	0.001	0.40	0	0.4	0.001	0.4	0.001	9.21	0.003	9.14	0.003	9.14	0.007	9.17	0.002
Labelling machine	33,197	30	1423	40	97.3	4.39	0.017	2.28	0.014	1.71	0.053	0.49	0.07	41.33	0.049	10.88	0.228	8.33	0.665	0.261	0.267
Crating machine	34,354	96	270	44	86.1	2.35	0.009	1.31	0.01	1.24	0.012	0.96	0.02	33.57	0.066	17.22	0.074	13.06	0.262	0.65	0.368
Palletizer	34,165	108	170	36	82.4	3.2	0.013	1.65	0.015	1.73	0.033	1.24	0.015	9.1	0.041	2.61	0.029	3.33	0.110	0.15	0.092
Crate washer	40,000	1	247	6	97.7	10.64	0.005	4.78	0.048	3.11	0.123	0.26	0.06	0.08	0.003	0.08	0.002	0.08	0.012	0.01	0
Mixer	36,000	1	-	-	-	25.78	0.206	23.47	0.135	1.92	1.412	0.97	1.365	0.45	0.011	0.03	0.004	0.07	0.064	0.1	0.022
Product heating [1]	36,000	1	-	-	-	1.83	0.015	0.995	0.024	0.995	0.024	0	0	0.7	0.128	0.7	0.128	0.7	0.128	1.23	0.197
Container transport [2]	-	-	-	-	-	12.32	1.794	-	-	1.95	1.385	1.24	0.066	-	-	-	-	-	-	-	-
Crate transport [2]	-	-	-	-	-	25.36	0.245	-	-	19.749	0.707	2.97	0.515	-	-	-	-	-	-	-	-
Pallet transport [2]	-	-	-	-	-	3.30	0.091	-	-	2.35	0.119	1.03	0.087	-	-	-	-	-	-	-	-

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2.4 Publication IV – Simulation of the batch-oriented production of the brewery and holistic hybrid simulation

Bär, Raik; Schmid, Sebastian; Zeilmann, Michael; Kleinert, Joachim; Beyer, Karsten; Glas, Karl; Voigt, Tobias. **Simulation of Energy and Media Demand of Batch-Oriented Production Systems in the Beverage Industry**. Sustainability 2022, 14(3), 1599; DOI: 10.3390/su14031599

Large brewery groups are setting ambitious targets with regard to their sustainability goals. As the production of beer is one of the most energy-intensive processes within the food and beverage industry, there is particular potential for increasing energy efficiency. Rising energy and electricity costs are a challenge, especially for small and medium-sized breweries, for which there are special barriers.

This paper presents an extended approach for the prognosis of the energy and media demand of the batch-oriented production within the brewery. Based on the already presented metamodeling approach and on the extension of the data structure an approach for the determination of simulation-relevant parameters as well as the automatic simulation model generation from a configuration file for the batch area of breweries is presented. Extensive measurement recordings within a brewhouse were performed to generate a comprehensive model with recipe-specific parameters and detailed production plans. Within the scope of this work, a simulation environment was further developed to represent the batch-oriented operation such as the brewing process and the simulation model was generated automatically. An extensive validation of the electrical and thermal energy demand of the brewhouse for three validation periods is presented and overall a good fit could be achieved. In combination with the preliminary work, the holistic simulation of the batch-oriented and discrete operation production within the brewery is presented and discussed by the example of a brewhouse and a beverage bottling plant. The whole method proves to be a good opportunity for comprehensive analysis with regard to the energy and media demand in the beverage industry

Contributions of the doctoral candidate (CRediT):

Conceptualization; methodology; software; validation; formal analysis; investigation; data curation; writing - original draft; visualization; project administration;

sustainability

MDPI

Article

Simulation of Energy and Media Demand of Batch-Oriented Production Systems in the Beverage Industry

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Abstract: The global brewing industry is facing enormous environmental challenges and is urgently required to produce sustainably and efficiently. The rising costs of energy and electricity are forcing small and medium-sized breweries in particular, which are confronted with barriers such as lack of capital and know-how, to make substantial changes. This article presents an extended approach to prognose the energy and media demand for batch-oriented production of a brewery. Therefore, based on a modeling editor as well as a standardized data structure and an approach to determine the simulation-relevant parameters, a solution for fast and easy model generation was developed. Extensive measurement recordings within a brewhouse were performed to create a comprehensive model with recipe-specific parameters and detailed production plans. A simulation model can be generated automatically from a configuration file in a simulation environment that has been extended to include the mapping of batch-oriented operation. A validation is presented and a maximum deviation of the electrical and thermal energy demand of 1–2% is achieved. In combination with a preliminary work, the holistic simulation of the complex combined production of batch-oriented and discrete operation within the brewery is presented and allows comprehensive analysis as well as optimization towards sustainable production.

Keywords: modeling; simulation; energy and media demand; validation; brewing industry

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1. Introduction

Not least due to the publication of the UN Sustainability Goals, companies are particularly required to produce sustainably [1]. The rising prices for energy and electricity are also forcing companies to act to continue to succeed in the market and to meet the demands of their customers. German companies are particularly affected by high energy and electricity prices [2]. The cost-driven food and beverage industry ranks third among the industrial sectors with the highest energy expenditures [3]. Beer production in particular is one of the most energy-intensive production processes in the food industry due to numerous heating and cooling processes in the brewhouse, numerous pumps and motors for material movement, and packaging and filling processes [4,5]. Large brewery groups are pursuing ambitious goals with regard to their sustainability, proclaiming targets such as CO_2 neutrality and halving water consumption by 2040 [6–8]. Thus, these efforts naturally also affect the supplying plant and mechanical engineering industry [9,10]. In particular, small and medium-sized companies (SMEs) in the beverage industry are urgently required to produce sustainably and energy-efficiently in order to withstand the enormous competitive pressure [11]. However, especially for SMEs, there are barriers such as lack of capital, know-how, and data and information from production to achieve efficient and sustainable production [12]. IT-supported measures such as simulation analysis represent an opportunity to uncover optimization potential and can thus contribute to energy efficiency and sustainability. The advantages of simulation lie precisely in the representation of complex processes, which can also influence each other [13] and in the testing of possible measures by adapting the models without influencing or interrupting real production [14]. However, it is precisely the creation of the simulation model and the determination of the parameters required for the simulation which are the main challenges in simulations. In addition, simulation studies are usually associated with high costs and require a high level of expertise [15]. There are some approaches described in the scientific literature for using simulation to improve energy and media efficiency in breweries. However, these are limited in terms of some factors and barriers and allow only limited holistic analysis. In a previous paper, the authors describe a solution approach of modeling and automatic simulation model generation for the packaging or bottling area of the brewery and elaborate on the relevant literature [16].

Mignon and Hermia [17] describe for the first time the simulation of several brewhouses using the software BATCHES, a program for the simulation of batch and semi-continuous processes. The aim of the work is, on the one hand, to investigate the brewhouses with regard to their design and, on the other hand, to reduce the energy demand by adapting the process. Furthermore, using the same tool, it was determined how measures can contribute to reduce the peak loads of the steam consumption in the brewhouse [18]. Adjusting the production schedule can also contribute to reducing peak loads [19]. Muster-Slawitsch et al. [20] explain the importance and methods of correctly modeling the brewing process. Areas considered include the heat-intensive thermal processes of the brewhouse and the cooling load within the brewery. In both areas, real data obtained are compared to data modeled using mathematics. The simulation of a brewhouse using neural networks to predict energy consumption is described by Bai and Pu [21]. However, only a very small database is used here and no concrete application of the method is described. Other work deals with brewery waste and wastewater recovery using modeling and simulation [22–24]. Special attention must be paid to modeling using petri nets or so-called reference nets and simulation based on them. Hubert et al. [25] model and simulate the cooling demand within small and medium-sized breweries. Based on an extensive database with different recipes, a forecast can be made over a period of almost one year and a detailed validation be presented. Another approach regarding the simulative investigation of the refrigeration demand during fermentation using multi-agent systems is described by Howard et al. [26]. A holistic hybrid approach, which covers several areas of the brewery, is described by Hubert et al. [27]. They present a simulation, also based on reference nets and Java programming, in the form of balance flows including factors such as the chemical oxygen demand of wastewater and energy management. The application of the method is discussed in more detail by Hubert [28]. Here, simulations take place within a brewhouse, the cellar area, for CIP plants as well as in beverage bottling. However, the use cases mostly refer to the equipment module level and include numerous factors, e.g., with regard to the raw material or process quality or the design of the equipment. Nevertheless, the electrical power requirements of pumps and the water requirements for CIP cleaning are also optimized. Furthermore, simulations using recipe specificity as well as stored historical production plans show where the largest consumption of electrical and thermal energy and water as well as the production of wastewater occurs. The validation of the method is limited due to the lack of a comprehensive database to map the consumption behavior in detail. In addition, due to its complexity and the required expert knowledge, the method offers only a limited possibility for breweries, especially for SMEs.

The approaches mentioned have in common that no simultaneous consideration of several subareas of the brewery takes place and thus no reference is made to the different production methods. In addition, they are predominantly limited to one type of energy and media. In particular, a recipe-specific consideration including a production plan takes place only in the works by Hubert et al. However, here, as in the other approaches, the database is described only to a limited extent or is not available and validation takes place only in part. Furthermore, a simple application of the presented methods is not given, since expert know-how or special software is required. These barriers pose particular challenges for SMEs in the brewing industry to increase their energy and media efficiency and to achieve sustainable production. A solution approach to overcome these challenges and barriers is presented by Bär et al. [16], but for the discrete packaging and filling area of the brewery. The present work takes up this approach and extends it to model and simulate the area of batch-oriented operation within the brewery with respect to its energy and media consumption.

This work presents an approach to the automatic generation of simulation models on the basis of an already presented modeling approach [29] and for the determination of simulation relevant parameters. Therefore, an extensive database was obtained by data measurement campaigns in the brewhouse of a medium-sized brewery. An overall model of the brewhouse with several recipes with specific parameter sets as well as with production schedules was created and, based on the configuration file of the modeling editor, a simulation model was automatically generated in a simulation environment, which was extended by the simulation of the batch-oriented operation. The simulation of the batch-oriented mode of operation is described in detail using the example of the brewhouse, and a detailed validation is presented. Furthermore, the holistic simulation of a complex production system consisting of the batch-oriented and discrete mode of operation is shown in the form of a use case by mapping the brewhouse and a beverage bottling plant in the simulation.

2. Brewhouse Investigated

Beverage production is divided into two fundamentally different production modes. First, the batch-oriented production of the beverage by means of process engineering measures must be mentioned [30,31]. In this processes, the raw materials required for the product are processed into the final product in several individual steps, with the steps influencing each other consecutively [31]. The ISA-88 standard regulates the subdivision of a batch process into its subprocesses and also describes an outline for the physical plants and recipes [32] and is described in detail for the application of a brewery by Bär and Voigt [29]. Figure 1 shows the brewing process with the respective units divided into the hot and cold blocks. The brewing process starts with the milling of the malt. The malt grains are mechanically broken up and mashed with water in the mash tun. The mash is then heated in individual temperature steps with specific durations. In some cases, a mash pan is also used for further thermal decomposition by boiling part of the mash. In the lauter tun, solid-liquid separation of spent grains and wort takes place. The obtained wort is boiled in the wort kettle with the addition of hops. After a whirlpool is used to separate the hot trub, the wort is cooled down to pitching temperature in a wort cooler [33]. This represents the interface to the cold block. The cold wort is transferred to a fermentation tank with the addition of yeast. The yeast starts alcoholic fermentation and breaks down the fermentable sugars into ethanol and CO_2. After fermentation, the young beer matures by storing it at low temperatures. Most beer types are filtered or centrifuged before the finished beer is put into a bottling tank prior to bottling [34]. Beverage filling represents the second part of the production modes due to the discrete mode of operation.

The brewery under investigation is a medium-sized German enterprise producing roughly 300,000 hectoliters per year of bottom- and top-fermented beers operating around the clock. The brewhouse presented in this paper has a cast-out wort volume of 100 hl per brew and, except for one special feature, corresponds to the structure presented. Regarding wort boiling, a gentle boiling system is used. In this process, the wort is kept hot only in the wort kettle and, after separation of the hot trub in the whirlpool, the wort is re-evaporated by means of a flash evaporator. The advantage is a high degree of flexibility in the boiling process and an increase in the quality of the wort [35]. Hot water (approx. 160 °C) is used as heat transfer medium throughout the brewhouse.

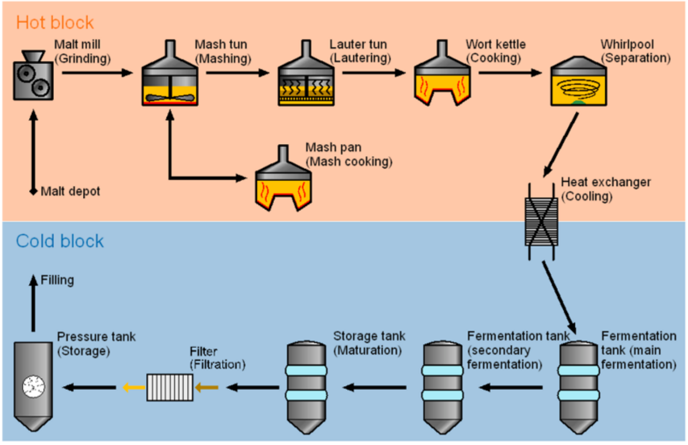


Figure 1. Brewing process divided into hot and cold blocks according to [34].

An overview of the consumption structures as well as the main consumers in the batch area of the brewery is given by Bär and Voigt [14]. It is important to note that the data described in the literature are in part subject to large fluctuations and are highly dependent on the size of the brewery, its modernity, and the product portfolio [14,36,37]. The most intensive processes in terms of thermal energy are boiling and mashing in the brewhouse. Electrical energy is required in the brewhouse mainly for the operation of the grist mill, mash and wort pumps, and motors such as for the agitator of the mash tun and mash kettle and for the lauter tun raking machine [14]. The cooling of the tank and the pumping over of the beer require enormous amounts of electrical energy. Recuperative thermal energy is obtained and used in numerous processes. For example, the water heated in the countercurrent heat exchanger can be used for mashing the subsequent brew [34]. A uniform procedure for recording energy and media consumption in the brewery has not yet been described. Only this would enable reliable comparability. A standardized approach for mapping and modeling production systems, such as breweries, with regard to energy and media consumption is presented by Bär and Voigt [29].

3. Data Acquisition

To meet the data needs of the underlying modeling approach, we propose a technique [38] to assess the energy and media consumption of brewing equipment at the unit level [39] and related to the brewing process. The brewery investigated, like most small and medium-sized breweries [40], lacks the prerequisite necessary to quantify and qualify energy and media consumption at such a low level of aggregation. Thus, the method framework is designed to be set up for a limited period, providing the entire equipment required to obtain the default modeling parameters. Measurement points are defined at the equipment module level and the control module level for each unit of the process cell brewhouse. In this context, electric motors to drive pumps for instance, constitute the equipment module level; the control module level is embodied by sensors (e.g., temperature sensors) and actuators (e.g., control valves). Where applicable additional data (e.g., recipe step sequences or motor switch signals) available from the brewhouse process control system (PCS) is used to derive the process model for each beer style and to qualify measurements, and are partly used to verify the measurements. To assess the energy consumption, suitable portable meters (PM) are selected for electrical energy (Janitza UMG 20CM channel branch circuit monitoring device; Janitza 20CM-CT6 operating and residual current monitoring module) and thermal energy (Flexim Fluxus F601 clamp-on energy flowmeter). Data from the PCS and PMs are recorded using a Windows-based computer running a Microsoft

SQL Server database, with a resolution of up to 1 data point × s^{-1} × parameter^{-1}. The PCS is connected via a local area network (LAN), whereas the PMs are connected via a programmable logic controller interface (PLC), as shown in Figure 2. The data format for a series of data points of a measurement point exported from database is as follows: measurement point ID—measured value—time stamp. The unit of each data point is retrieved from the PLC or the PCS. Correlation of the individual data points is facilitated employing a single system clock, even in the event of a non-equidistant recording.

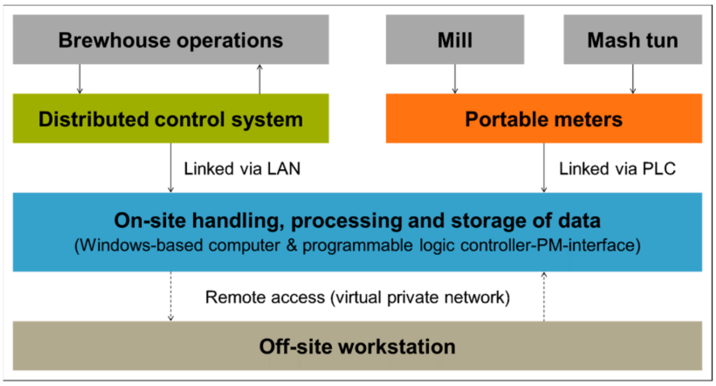


Figure 2. Quantification and qualification of energy and utility consumption at the unit level (according to [41]).

From milling the malt through to cooling the wort each unit of brewhouse was assessed, resulting in a total of 26 measurement points for electrical energy and a total of 6 measurement points for thermal energy. In addition, more than 100 parameters from sensors and actuators are incorporated. The measurements were divided into three consecutive series, each series covering a selected section of the brewhouse as well as energy types, and each covering a period of approximately 14–21 days).

MATLAB 2020b [42] software was used to prepare the raw data. During data import, the measured values were linearly interpolated over the entire measurement period of each data trace and normalized to equidistant time intervals of one second. The data were stored in an SQL database, which follows a generic and standardized structure as described by Bär et al. [16]. The data are divided into interval data and timestamp data. Interval data comprise the duration of a Process Operation of a unit, whereas timestamp data describe the consumption values at an exact point in time. The nomenclature and semantics of the data points correspond to the Weihenstephan Standards [43]. In addition, the database comprises tables containing units, data points and processes, subdivided up to the Process Operation. In addition, the production plan is imported. With the help of keys, it is possible to reference between the individual tables, which also enables easy expansion of the database. This data structure is used for the raw data as well as for the simulated data.

4. Modeling Approach

To map the energy consumption behavior of a plant in the beverage industry completely and in detail, a context-free approach in the form of a metamodel was developed [29] and applied in this work. A metamodel, which describes models as a superordinate instance, is presented based on four modeling pillars. In addition to the physical model, the process model, a recipe or article model and a production plan model are defined. The modeling approach is implemented in a graphical modeling editor, which ensures fast, simple and structured model creation. The modeling approach has already been applied in detail for the packaging and bottling area within the beverage industry and described [29].

The physical model of the batch area (e.g., brewhouse) includes all real existing units, such as a mash tun, which are placed and linked as building blocks on a surface, described by a coordinate system. In the process model, the running processes and their sublevels (according to ANSI/ISA 88 [39]) are defined for the batch area (see Figure 3). Starting at the Process level, individual Process Operations are modeled via the Process Stage level. The Process Operation level represents the consumption-relevant level, in which they can be freely defined. The modeling of the process model in the modeling editor is based on the modeling language Business Process Model and Notation Language (BPMN), and four essential basic building blocks, which describe “Filling”, “Emptying,” “Processing” and “Setup”, can be used. To define the sequence of the individual Process Operations, they are linked with arrows. The notation of BPMN makes it possible to depict the exact sequence of process steps across all three levels. The duration as well as the corresponding amount of energy and media required for the corresponding Process Operation are parameterized in the modeling editor. To simplify and speed up the modeling, required energy quantities can also be calculated. Factors can be used to describe the different energy and media efficiency of a unit as well as the share of recuperative energy.

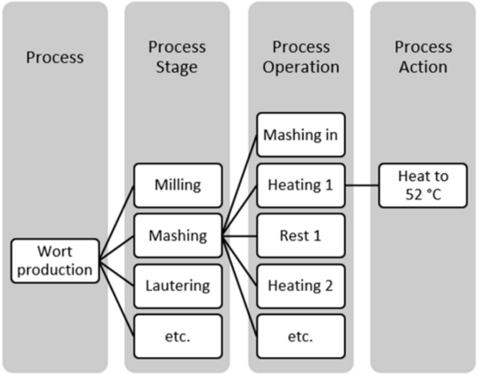


Figure 3. Division of the process model according to ANSI/ISA 88 [39].

Recipes are modeled by linking the Process Stages of a process model to units of the physical model, which increases the variability in the modeling and allows specific attention to be paid to the different product consumptions, but also to the differences in consumption of products in different Process Cells (e.g., brewhouse 1 and brewhouse 2). A process is modeled specifically for each recipe in the batch area. The production plan model covers all modeling columns with the definition of a flow chart, which contains the sequence of brews to be produced, as well as a matrix model for mapping the times between the individual brews of different recipes (brew cycle). In addition, a shift plan is stored to limit the total available time. This sets the framework conditions for the later simulation of the model. The modeling editor generates an XML configuration file which contains all simulation-relevant parameters and structures.

5. Energy and Media Consumption Behavior and Determination of Simulation Parameters

The energy and media consumption behavior of batch-oriented processes is described in detail by Mignon and Hermia [17] and Muster-Slawitsch et al. [20]. The energy and media consumption depend on the currently applied process. According to the subdivision of ANSI-ISA 88 [39], the modeling approach uses the level of Process Operations in the process model as well as the unit level in the physical model. For example, considerably more thermal energy is required in a “Heating” Process Operation than in a “Resting” operation. With regard to electrical energy, clearly different consumption levels can be identified, e.g., pump or agitator operation. The following method is used to determine the individual Process Operations, their durations, and their energy and media requirements. The subdivision of the processes into individual Process Stages is determined on the basis of the units used. The division of a Process Stage (e.g., “Mashing”) into Process Operations is based on the change in the consumption levels of the individual energy and media types. For this purpose, the data traces of the respective energy and media types of the individual consumers (equipment modules) of a unit or within a Process Stage are summarized and displayed graphically. The challenge in the definition of the Process Operations lies in the simultaneous consideration of the different energy and media types. If different consumption levels of different energy/media types overlap, they must be defined as further individual Process Operations. The start and end times of the Process Operations are derived manually and, in this case, stored in a SQL database following the presented data structure.

Figure 4 shows an excerpt of the course of the thermal and electrical energy consumption during the “Mashing” Process Stage. The Process Operations to be derived on the basis of the change in the respective power requirement can be seen in grayscale. The manual delimitation allows maximum and flexible granularity.

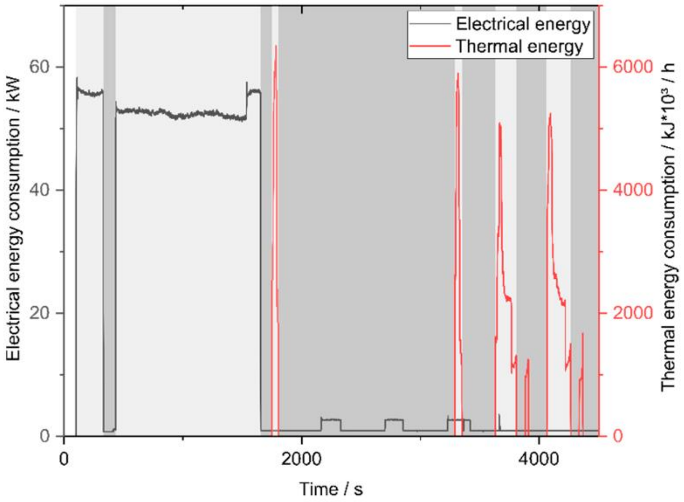


Figure 4. Example of the derivation of the individual Process Operations (highlighted in grayscale) based on the curves of the electrical and thermal energy demand for the Process Stages “Mashing” (section).

Based on the graphical plots of the electrical and thermal energy demand as well as the start and end times of the respective Process Operations, the required energy and media quantities can be determined by integration. Applications for this are common practice [44] and are used in various works [45,46].

The area under the data curve is determined using the trapezoidal rule (1). The numerical approximation of the integral of the function of the data curve is done by using several trapezoids of equal width. The width corresponds to one second in the present application.

$$\int_a^b y(x)dx = \frac{b-a}{2N} \sum_{n=1}^{N} (y\ (x_n) + y(x_{n+1})) \tag{1}$$

Since a unique consumption value y is assigned to each second value x in the data stored in the SQL database, the result is shown in (2).

$$\int_a^b y(x)dx = \frac{b-a}{2N}\sum_{n=1}^{N}(y(x_n)+y(x_{n+1})\ ) = \frac{b-a}{2N}[y(x_1)+2y(x_2)+\ldots+2y(x_N)+y(x_{N+1})] \quad (2)$$

By using equidistant time intervals, energy can be determined by integrating power in the time intervals. An equivalent procedure is followed with respect to thermal energy. With a corresponding scope of data, the consumption values can be statistically examined and evaluated for each Process Operation on a recipe-specific basis. For this purpose, in particular, the automated determination of the consumption data based on the manually recorded times by means of software is recommended. The average values of the individual durations and the required amount of energy/media can then be used to parameterize a simulation model.

6. Simulation Environment

All simulation studies were carried out using the time-discrete "PacSi" simulation environment developed by SimPlan AG, Dresden, Germany. The simulation software masters the discrete simulation of packaging processes [47] and was further developed in the context of this work for the simulation of batch and thus continuous processes in the beverage industry with regard to their energy and media consumption. In combination with discrete manufacturing in the packaging sector, which has already been described comprehensively with regard to the mode of operation, validation and with simulation experiments [16], the simultaneous simulation of holistic production systems, such as the brewery, has been made possible.

To represent batchwise production within the brewery (process areas: brewhouse, fermentation/storage/filter cellar) in the simulation environment, the following concepts of the necessary functionalities for the extension of the simulation system were developed and fully implemented. A fundamentally new development is the automatic simulation model generation based on the XML exchange file. The building blocks in the modeling editor are assigned to a newly developed batch building block within the simulation. The coordinate system and the links of the elements can be used to reformulate the logical structure of the plant. In contrast to the discrete domain, the batch module is based on a time-dependent specification of the individual Process Operations. This means that the Process Operations modeled in the process model are executed one after the other and the corresponding parameterized energy/media consumption level is applied for the respective duration of the Process Operation. The programmatic implementation in the batch module of the simulation environment follows the sequence "Fill—Process—Empty." At the runtime of the simulation, the corresponding parameters, such as the duration of the Process Operation and the corresponding consumption values, are loaded and reformulated if necessary and the simulation model is parameterized continuously. A special feature here is the integration of a production plan, i.e., the sequence of different recipes. This is mainly solved for the main source, the element in which material is released in the simulation, by storing the non-production times and the times between the individual recipes and their specific article number. This indexing allows an element-specific parameter change and thus enables the recipe-specific simulation within the production plan. The simulation of each Process Cell takes place in its own interface within the simulation, but several interfaces can be active at the same runtime, thus enabling the holistic simulation of production systems in the beverage industry. To be able to analyze simulation tests in a flexible granularity and with regard to different sizes, the simulation results are stored in the presented database structure in an SQLite database. A fast and simple evaluation is carried out by a specially developed evaluation software in MATLAB 2020b AppDesigner [42], which allows a recipe- and plant-specific determination of the required energy and media quantities for each of the Process Operations.

The evaluation software connects to the results database and dynamically determines the respective process elements and units as well as the associated data points. A specific query code is generated to determine the consumption data within the respective time intervals of the Process Operations. The structure stored in the database makes it possible to compile the data into an overall picture. The procedure is implemented in user-friendly interfaces, through which the user is intuitively guided. The results are finally output in tabular form including all data.

7. Verification, Validation & Use Case Demonstration

The verification and validation of the method are intended to underpin the reliability of the model creation, the simulation and the validity of the simulation results and to serve as proof of the correct functioning. Especially with regard to possible resulting decisions in the implementation this is essential. The verification includes the examination of the conversion of a model such as the model in the modeling editor, into another model such as the simulation model. Therefore, the generated model was checked manually for correctness with regard to the topology, the elements and their correct connection. During the simulation run, the different parameter sets of the recipes were regularly checked and compared with the values within the model in the modeling editor. To check the results of the simulation and thus its correct functioning, a simulation run was evaluated manually using the freeware HeidiSQL_11 [48], which allows manual access to and viewing of SQLite databases, on the one hand and using the self-developed evaluation tool on the other.

Validation is to check the correct functioning of the model for the specific application purpose in the simulation compared to reality [49]. In the present case, the validation refers to the simulation of batch-oriented production in the brewhouse of a brewery. The measured and simulated consumption values are compared within the validation periods, according to Al-Hawari et al. [50], with the measured value representing the reference value.

The application of the combined simultaneous simulation of batch and discrete operation is to be demonstrated with the help of a use case. For this purpose, the method presented in this paper is combined with the method of the discrete packaging/bottling area of the beverage industry [16] and shown on the basis of the hybrid simulation of a brewhouse and a beverage bottling plant.

8. Results

8.1. Validation Periods and Simulation Parameter

Three different time periods, defined within the respective time periods of the measurement data recording, of the presented brewhouse are available for the validation of the simulation (see Table 1). In the first two measurement periods, different processes and thus units were examined and measured with regard to the electrical energy demand. In the third measurement period, the entire brewhouse and its processes were examined with regard to thermal energy consumption. Each of the periods covered a different sequence of brews with a combination of three different recipes over a period of 140–170 h.

Table 1. Overview of the validation periods of the brewhouse including the brew cycle (W—Wheat, P—Pilsner, L—Lager).

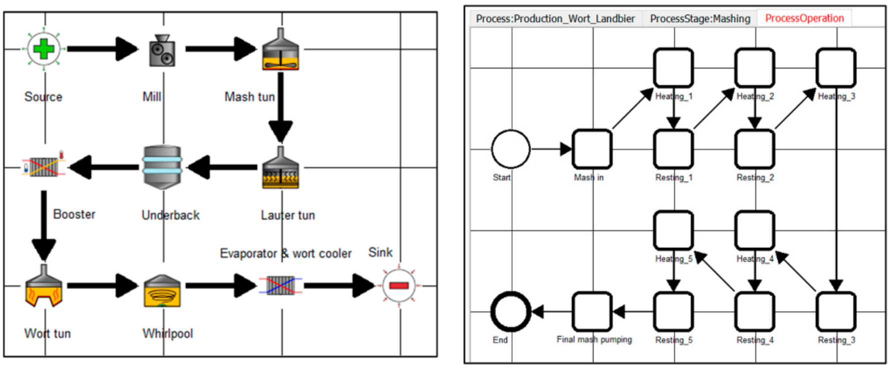
Validation Period	Duration/Number of Brews	Brew Cycle	Type of Energy/Media Investigated	Process Stages
1	168.83 h/71 brews	13× W, 19× P, 1× L, 18× W, 14× L, 1× P, 5× L	Electrical energy	Milling, Mashing, Lautering
2	139.88 h/60 brews	10× P, 1× L, 1× P, 1× W, 7× P, 10× L, 1× P, 9× L, 7× P, 13× W	Electrical energy	Heating up wort, Keeping heat, Vaporization & cooling
3	143.9 h/60 brews	17× L, 1× P, 18× W, 24× P	Thermal energy	Whole brewhouse process

The number, times as well as energy and media quantities of the individual Process Operations were determined recipe-specifically. This was done semi-automatically by implementation in self-programmed software in MATLAB R2020b [42]. The start and end times of the Process Operations were derived manually and the time stamps were automatically transferred to the interval table of the database. For more precise delimitation, brew logs, step chain logs of the individual recipes and historical PLC data, such as valve cycles, were used. The software determines the resulting energy and media quantities of the Process Operations according to the method presented in chapter 5.

The simulation-relevant parameters were determined for measurement periods 1 and 2 in the following number for each recipe: 12× Wheat, 15× Lager, 15× Pilsner. When the thermal energy demand in measuring period 3 were recorded, 10 brews per recipe were evaluated. Thus, statistically validated simulation parameters of the individual Process Operations could be determined. Table A1 shows the Process Operations and the associated simulation parameters for the Pilsner recipe. In total, there are about 600 parameters for the entire simulation model with three recipes. The times between the individual brews (brew cycle) of the different recipes were determined as the mean on the basis of all the data and transferred to the model. The basis for this is the filling and startup of the malt mill.

8.2. Model of the Brewhouse

The brewhouse investigated in this work was modeled in the presented modeling editor. Figure 5a shows the physical model of the brewhouse consisting of the units as described in chapter 2. The special features of the modern boiling system include the pre-run tank, wort preheating (booster) and post-evaporation by the gentle boiling system. Therefore, the wort is kept hot in the wort kettle. The source serves as the interface to the upstream malt store and the sink as the interface to the fermentation tanks, corresponding to the transition to a possible further process cell, the cold block of the brewery. In the Wheat recipe, a decoction mashing process is used, i.e., the physical breakdown of the starch by boiling up a partial mash. A mash pan is used for this purpose. To simplify the model, the parallel process step of mash boiling was implemented energetically in the "Mashing" Process Stage in the mash tun. Figure 5b shows the process model on the Process Operation level within the Process Stage "Mashing" for the process of wort production for the Lager. The arrows define the respective sequences of the processes, respectively the linking of the units. The start and end elements of the process model represent the connection to the start and end of the respective higher Process Stage.



(**a**) (**b**)

Figure 5. (**a**) Model of the presented brewhouse and (**b**) model of the Process Stage "Mashing" ("Lager") (adapted from [29]) in the modeling editor.

In the recipe model, the individual Process Stages within the process models were linked to the units of the physical model and additional information, such as the brew size, was indicated. The production plan was parameterized in each case as shown in Table 1. In addition, the times of the brewing sequence, the shift times and the respective start time of the simulation run were defined as the day of the week and the time of day.

8.3. Validation Results

8.3.1. Model and Simulation Verification

As in the previous work of the authors [16], the verification of the automatic model generation in the simulation environment based on the XML configuration file resulting from the modeling editor was performed manually. In addition to verifying the correct generation of the simulation model, all parameters of all recipes were manually checked. In particular, the correct sequence of the individual Process Operations and their durations and energy/media consumption levels were examined. In addition, the sources, which represent the inflow of the main stream and thus the production schedule, were checked for correct functioning and production quantities and brew cycle times. The verification was performed continuously with the development process of the simulation environment and could be completed successfully.

8.3.2. Validation of the Brewhouse Energy and Media Demand

The validation of the brewhouse electrical energy demand is divided into two periods, but in each case all processes were simulated with the complete parameter sets. This also applies to the validation of the thermal energy demand. In all three periods, the brew number is reached according to the periods in reality and a respective maximum time deviation of 1% could be determined. First, the curves of the electrical and thermal energy demand for one brew and for selected validation periods as well as detailed sections of them are presented. Subsequently, the validation and real values of the individual Process Stages as well as the entire periods are listed and their percentage deviation is shown.

Figure 6 shows the comparison of the simulated electrical consumption curve, which results from the determined parameters of the model, with the measured consumption values of a combined brew. Due to the division of the measurement exception of the electrical energy demand, the measured data curve consists of two different brews. It can be seen that the large consumption peaks caused by the pumps during “Mashing in” and the pumps in the Process Stages “Vaporization and Cooling” are reflected especially well. Small consumption peaks, which sometimes only occur for a few seconds (see beginning), cannot be reproduced. The time offset results from the mean values of the Process Operation durations in the parameterized model.

Figure 7 shows the course of the electrical energy demand in validation period 1. The consumption curves of the individual processes and the cumulative total consumption are shown. The starting production at the beginning of the simulation, in which only the “Milling” and “Mashing” processes are initially active, can be seen. Since the lauter tun represents the bottleneck of the brewhouse, the times of the brew cycle are designed for the optimum utilization of this unit. As the simulation time progresses, the demand curves overlap more and more and several brews are active in different processes in the brewhouse at the same time. This sometimes results in very high demand peaks.

Figure 8 shows a detailed section with the different demand curves for electrical energy, which reflect the unit measured for a Process Stage or Process Operation. In addition, the associated Gantt chart for equipment occupancy on the unit level is presented. Due to the parallelism of processes such as simultaneous “Mashing” (e.g., pump during mashing and pump during boosting) and “Vaporization and Cooling”, enormous consumption peaks sometimes occur. This also causes the two extremes, in which both Process Stages of different recipes overlap (see Figure 7).

The validation of brewhouse thermal energy consumption is based on the continuous measurement of the individual units within a period of time. Figure 9 shows the comparison of the real measured and simulated consumption of thermal energy during one brew. The times of the Process Operations and the consumption parameters of the simulation are based on the mean values from the data acquisition. The two curves agree well, although short peaks, sometimes lasting only a few seconds, cannot be accurately represented by averaging the real consumption curve.

Figure 10 shows the course of the thermal energy demand in validation period 1. The consumption curves of the individual Process Stages and the cumulative total consumption are listed. No thermal energy is required for the Process Stage "Vaporization and Cooling", but is generated recuperatively via heat exchangers. This energy is reused within the production system. The constantly repeating consumption profiles, depending on the recipe, can be seen.

Figure 11 shows a section of the thermal energy demand as well as the associated equipment occupancy chart in detail. The individual process days and the Process Operations in which thermal energy is required are marked. A total demand curve is also shown. The "Vaporization and Cooling" Process Stage is not included in the overall analysis.

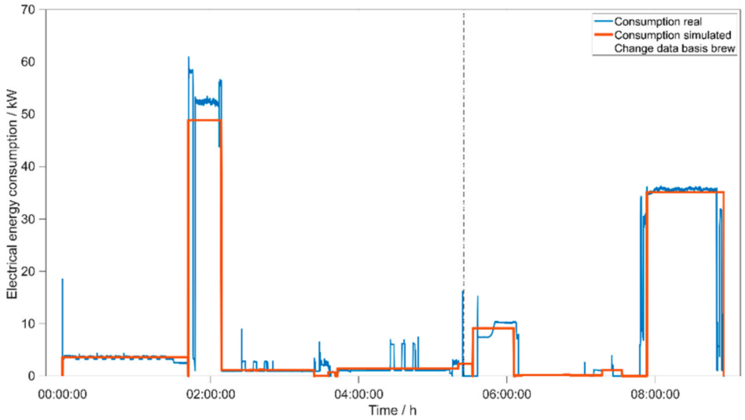


Figure 6. Comparison of the electrical energy consumption [kW] of one brew (real & simulated) "Lager".

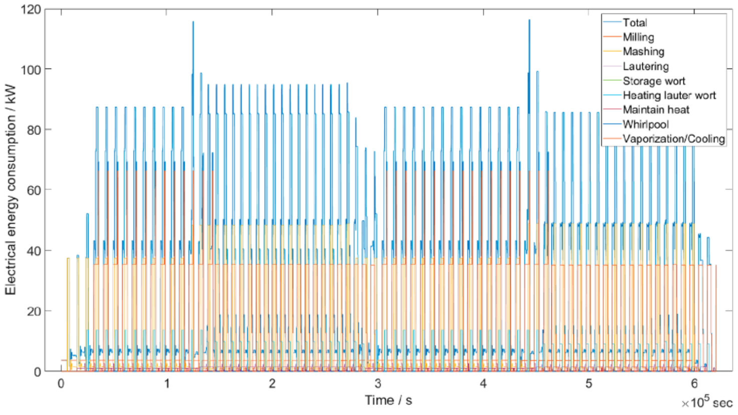


Figure 7. Electrical energy consumption [kW] of all processes of the brewhouse in validation period 1.

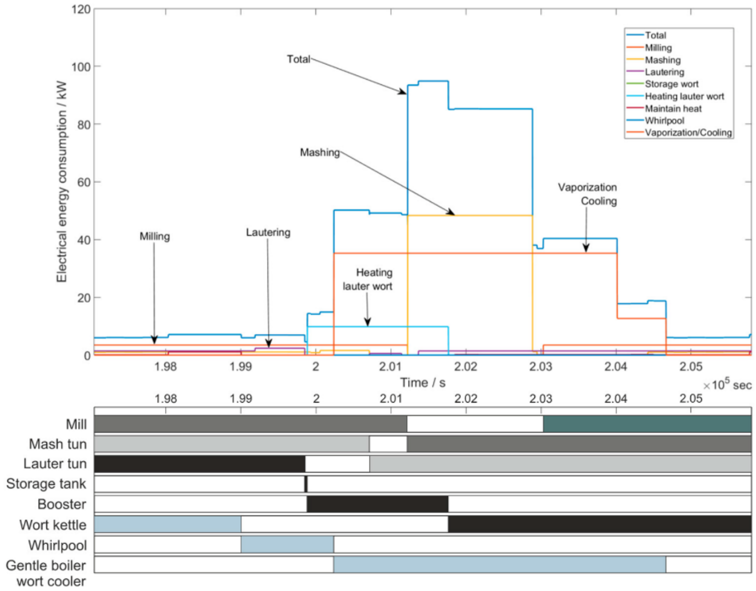


Figure 8. Detailed electrical energy consumption [kW] of all processes of the brewhouse in validation period 1 incl. the equipment occupancy in a Gantt chart.

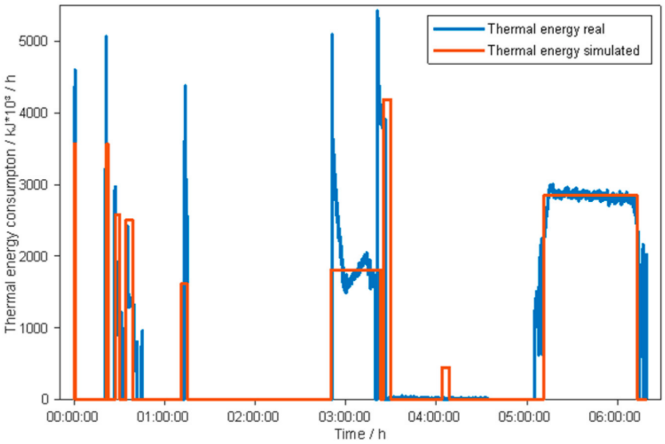


Figure 9. Comparison of thermal energy demand [kJ/h] of one brew (real & simulated) "Lager".

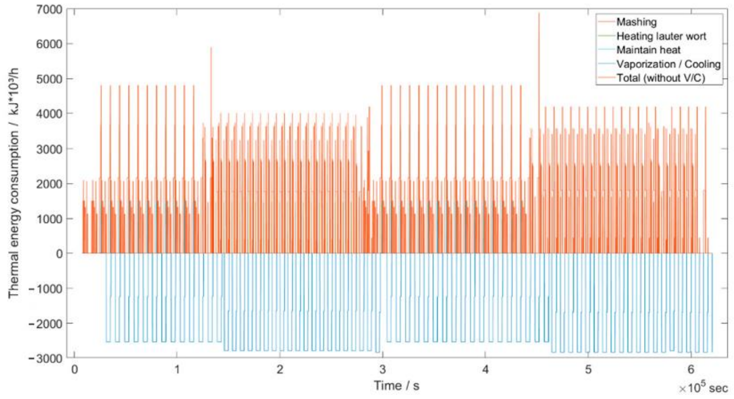


Figure 10. Thermal energy consumption [kJ/h] of all processes of the brewhouse in validation period 1.

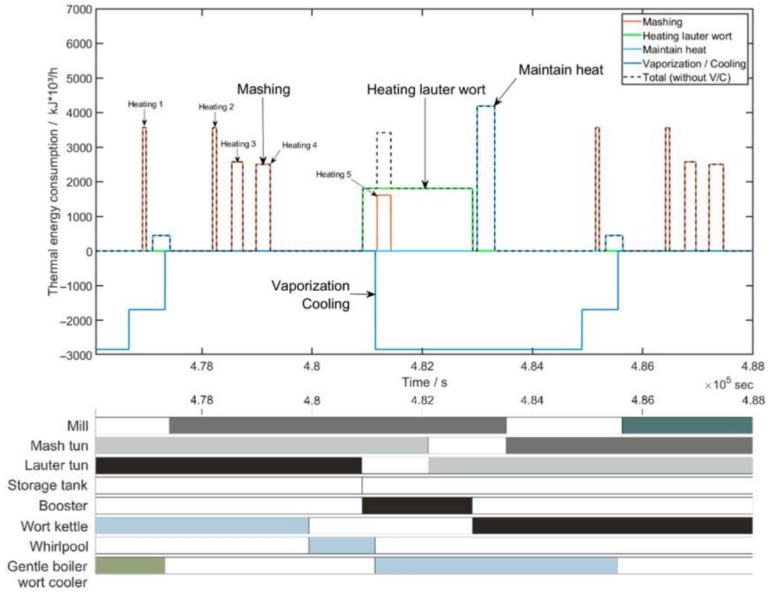


Figure 11. Detailed thermal energy consumption [kJ/h] of all processes of the brewhouse in validation period 1 incl. the equipment occupancy in a Gantt chart.

Table 2 shows the validation of the electrical and thermal energy demand by the comparison of the simulated and measured consumption quantities and their percentage deviation. The validation is carried out generally and specifically according to the division of the Process Stages and the respective recipe. Due to the divided measurement recordings, the respective values refer to the corresponding measurement and validation periods. The values also differ in the number of brews, the recipes and the sequence. The two Process Stages "Wort Storage" in the underback and "Separation" in the whirlpool are not listed in the table, as no energy or media consumption was assigned to these steps. The values were determined by one simulation run per time period since, due to the lack of stochasticity of the duration of the individual Process Operations, a multiple simulation would not show any deviating consumption values.

Table 2. Validation results for electrical and thermal energy demand (simulated, measured & percentage deviation) for all Process Stages and for all recipes in the three validation periods.

Validation Period	Unit	Process Stage	Electrical Energy [kWh]											
			Lager			Pilsner			Wheat			Total		
			Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]
1 (20× L; 20× P; 31× W)	Mill	Milling	121.94	119.61	1.95	115.05	115.59	−0.46	181.33	176.88	2.51	418.32	412.08	1.51
	Mash tun/pun	Mashing	467.59	475.44	−1.65	472.61	500.91	−5.65	724.16	753.63	−3.91	1664.36	1729.98	−3.79
	Lauter tun	Lautering	57.02	56.88	0.25	54.38	54.96	−1.05	81.79	81.20	0.74	193.19	193.03	0.08
2 (20× L; 26× P; 14× W)	Booster	Heating up wort	101.13	100.03	1.10	133.53	124.12	7.58	77.50	76.54	1.25	312.17	300.70	3.81
	Wort kettle	Keeping heat	10.08	8.71	15.71	12.44	11.86	4.85	5.32	5.80	−8.23	27.84	26.37	5.56
	Gentle boiler, wort cooler	Vaporization & cooling	776.22	738.60	5.09	1021.32	970.50	5.24	539.42	542.93	−0.65	2336.96	2252.03	3.77
	Brewhouse	Total	1533.98	1499.27	2.32	1809.34	1777.95	1.77	1609.52	1636.98	−1.68	4952.84	4914.20	0.79
			Thermal Energy [kJ]											
			Lager			Pilsner			Wheat			Total		
			Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]	Sim.	Meas.	PD [%]
3 (17× L; 25× P; 18× W)	Mash tun/pun	Mashing	9.73×10^6	9.10×10^6	6.98	1.44×10^7	1.38×10^7	4.62	2.36×10^7	2.22×10^7	6.55	4.78×10^7	4.50×10^7	6.04
	Booster	Heating up wort	1.70×10^7	1.56×10^7	8.93	2.31×10^7	2.38×10^7	−2.89	1.58×10^7	1.55×10^7	1.73	5.59×10^7	5.49×10^7	1.78
	Wort kettle	Keeping heat	5.44×10^6	5.45×10^6	−0.15	7.89×10^6	7.89×10^6	0.01	6.42×10^6	6.05×10^6	6.13	1.97×10^7	1.94×10^7	1.87
	Gentle boiler, wort cooler	Vaporization & cooling	5.56×10^7	5.26×10^7	5.65	8.08×10^7	7.98×10^7	1.16	5.41×10^7	5.54×10^7	−2.30	1.90×10^8	1.88×10^8	1.40
	Brewhouse	Total	8.78×10^7	8.28×10^7	6.03	1.26×10^8	1.25×10^8	0.70	9.99×10^7	9.91×10^7	0.82	3.14×10^8	3.07×10^8	2.18

In the area of electrical energy, a very small deviation of 0.8% can be determined in the overview. The largest deviation concerns the process step “Keeping heat” within the wort kettle. However, this Process Stage has a small share of the total demand, 0.56%. The deviations are also reflected in the recipe-specific analysis. Furthermore, the steps “Mashing”, “Heating up Wort” and “Vaporization & Cooling” show similar deviations in the range of 3.8%. In these processes, electrical energy is required mainly for pumps to transfer the brew, which covers a similar volume across the recipes. Some of the largest deviations in the values from validation period 2 are achieved for the Pilsner recipe. This is due to the relationship between the basis of the number of brews measured in the measurement period, which vary in the range of electrical energy, versus the number of brews in the validation period. In general, it can be concluded here that a larger number of brews examined in the parameter determination leads to more exact agreements within the validation periods. Nevertheless, very small deviations between the measured and simulated values can be observed uniformly in relation to the respective recipes.

In the area of thermal energy, the largest deviations exist for the “Mashing” Process Stage. This is clearly due to the high number of Process Operations (12–14) in the mashing and the associated inaccuracy in parameter determination due to the definition of the time limits. Especially in the Lager recipe, high deviations occur in the “Heating wort” step due to the booster. In combination with the deviations in vaporization/cooling, this results in a total deviation of 6% for this recipe. This phenomenon is due to the low database for “Vaporization & Cooling”, as there were also difficulties with the measurement during operation. The Process Stage “Keeping heat” also shows high deviations for the recipe Wheat, but accounts for only 6% of the total thermal energy requirement. The remaining simulated values agree very well with the measured values and a maximum deviation of 2% is achieved in each case. Overall, this results in very small deviations for the Pilsner and Wheat recipes and a total percentage deviation of 2.2% is achieved.

8.3.3. Use Case

In a previous study, a use case was developed for the simulation of a brewhouse with regard to the reduction of peak loads of electrical energy by adjusting the brew cycle times. A reduction in peak loads of up to 32% was achieved [29].

For the first time in the scientific literature, the holistic hybrid simulation of batch-oriented and discrete operation is presented. For this purpose, the presented method for the simulation of the batch area of the brewery is used in combination with the already presented approach for the simulation of packaging and bottling plants [16]. The presented brewhouse and a returnable glass beverage bottling plant were modeled together in the modeling editor. The simulation model was automatically generated in the simulation environment based on the XML configuration file.

The resulting model comprises two process cells (batch-oriented brewhouse and discrete beverage bottling plant) with three recipes and four filling articles. All parameters were evaluated on a recipe/article-specific basis and the model was parameterized accordingly. In addition, a corresponding shift plan was defined for both areas to define the daily start and end times. Production in the brewhouse is round the clock, whereas in the bottling area production takes place from Monday 7:00 am to Saturday 8:30 am. Toward the end of the simulation period, a weekend is therefore depicted. In addition, the brew cycle times and changeover times between the filling articles are stored for both process cells. The simulation covers a total time of 7.5 days, starting at Sunday 10 pm. Figure 12 shows the course of the electrical energy demand of the brewhouse and of the beverage bottling plant and the sum of these. The delayed start-up of the beverage bottling plant due to the limited shift schedule for this process cell can be seen clearly. Furthermore, the resulting total consumption and the resulting peaks due to the overlapping of many individual electrical energy consumers can be seen well.

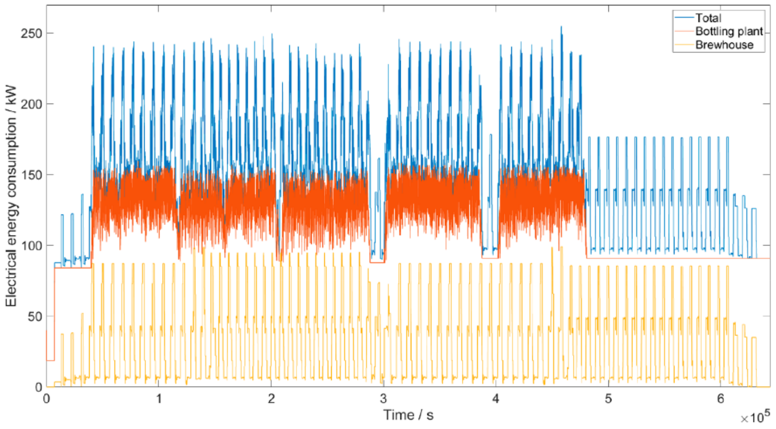


Figure 12. Electrical energy consumption of the combined simulation of the brewhouse and the beverage bottling plant.

The use case shows that the entire method is suitable for a holistic analysis and forecast of the energy and media consumption of plants in the beverage industry and can simulate any number of plants of the batch-oriented as well as the discrete operation mode. The method enables holistic energetic consideration and opens numerous possibilities for carrying out experimental tests to increase energy and media efficiency on the basis of numerous factors.

9. Discussion

Due to the structured subdivision of plants and the corresponding processes according to ANSI/ISA-88 [39], the data acquisition procedure is well suited for transferability to any batch-oriented production operation. Although standardized procedures for collecting data on energy and media consumption are available, such as for packaging machines [51], no approach has yet been described for the batch-oriented production area of the brewery. Since the collection of data is very time-consuming, a solution is especially needed for the application of a standardized determination of consumption parameters.

Due to the flexible subdivision of the Process Operations, energy and media consumption behavior can be mapped in any granularity. The effort of manually defining the start and end times of the Process Operations has optimization potential. This effort can be automated if reliable raw data are available, for example relating to the sequence of the step chain. Also conceivable is the automatic detection of peaks, although the definition of a peak and the relevance of a peak remain open. Nevertheless, the one-time manual delimitation of Process Operations on the basis of consumption curves and with the help of context data such as brew logs, step chain logs and other PLC data make it possible to precisely delineate the individual Process Operations. On the basis of the standardized data structure, the simulation-relevant, recipe-specific consumption parameters can be calculated automatically in a standardized way using a self-developed tool in MATLAB R2020b [42]. This enables the comparability of the simulation parameters. The parameters consistently show very low confidence intervals and can therefore be considered reliable. The parameter determination tool is structured via graphical interfaces and can thus be used without specific prior knowledge or requirements.

The model of the brewhouse with all parameters and the production plan model were created in a structured and standardized manner in the graphical modeling editor, which is based on modeling columns. Due to its ease of use, the model can be created quickly and checked for correctness with the help of help functions and automatic checks. Compared to time-consuming manual parameter determination and simulation model creation, which in this case require several weeks, the present simulation model can be created within a few days with the help of the parameter determination, the modeling editor and the automatic simulation model generation. The prerequisite for this is a reliable database. Fast model creation overcomes a significant barrier for companies in the beverage industry. A novelty is the integration of a production plan with different recipes, which are represented by different parameter sets. The automatic generation of simulation models of the batch-oriented mode of operation can be shown on the basis of the XML configuration file as exemplified by the used simulation environment. Since the configuration file contains all simulation-relevant information, the automatic model generation is transferable to any simulation environment.

Based on three different time periods of the brewhouse, an extensive validation can be carried out to prove the suitability of the entire method. The simulated values were compared with the real measured values and the percentage deviation was determined. The evaluation was carried out both overall and recipe-specific. The validation is limited to the electrical and thermal energy consumption of the brewhouse of a brewery as no measured data were collected for other types of energy and media or other areas such as fermentation/storage cellar and filtration. In all periods, the production plan was processed as specified and the simulated time deviates only very slightly from the production time required in reality.

The direct comparison between the simulated course of a brew and a real brew shows well the agreement of the temporal and quantitative demand of electrical and thermal energy. The values of the simulated course result from the mean values of the determined times and consumption parameters of the individual Process Operations and are therefore repeated for each recipe. This explains the time deviations due to the slight shifts of individual consumption peaks in both figures. There are also individual peaks which are not represented by Process Operations and are therefore disregarded. Most of these peaks occur only very briefly (a few seconds) and also have only a minor effect on the total electrical energy demand. In the area of thermal energy, the short maximum peaks are only partially mapped due to the averaging of the consumption value over the duration. The figures of the detailed electrical and thermal energy curves of the individual process stages, together with the unit occupancy Gantt charts, show well how the consumption peaks are formed. In reality the occupancy of two consecutive units overlaps due to the simultaneous emptying and filling of the vessels. In the simulation this is simplified by a direct transition. In the brewhouse, several brews are usually active because of the bottleneck, the lauter tun, which leads to a simultaneity of Process Stages. Especially when different recipes follow one another, very high consumption peaks can sometimes occur due to overlapping. A use case already presented deals with the shifting of consumption peaks by adjusting the times of the brew cycle in the production plan [16]. The overall view of the consumption curves in validation period 1 illustrates this. The functionality of the simulation is clarified by the representation of the complex process structure, which is significantly influenced by the production plan. This offers a good opportunity for companies in the beverage industry to depict the total demand of their production facilities and to test possible efficiency improvements. The thermal energy curve in particular illustrates how much thermal energy results in the brewing process and can be further used as recuperative energy. This is state of the art and is discussed in numerous publications in the form of sources and sinks as well as heat cycles and is not the subject of further investigation in this work.

The numerical comparison of the validation is performed in the granularity of the Process Stages and the recipes. The three validation periods have a similar duration, different sequences of the brews and a varying number of brews. The brews, which serve as the database for parameter determination, are outside the validation periods. This ensures that the method of parameter determination is also included in the validation. The total values refer to the sum of the Process Stages within the respective recipe due to the split measurement periods. Overall, a very good agreement of the electrical energy demand is achieved. Most of the consumptions concerning the Process Stage “Keeping heat” can be disregarded due to their small share of the total demand. The “Vaporization & Cooling” Process Stages, together with “Mashing”, have the greatest influence on the total requirement and also sometimes show the highest deviations. This goes hand in hand with the number of Process Operations within these Process Stages. It can therefore be concluded that, in conjunction with the number of brews investigated, the division into Process Operations has a significant influence on the deviations. A larger database as well as the automated recognition of the Process Operations would remedy this situation. This also applies to the deviations of the thermal energy values. Especially for heating processes, a small database is a challenge, since numerous external influences can affect the required energy. Nevertheless, very small deviations are achieved overall and for the Pilsner and Wheat recipes.

A novelty describes the combined simulation of the batch-oriented and the discrete mode of operation in the use case. The challenge here is the simultaneous representation of the time-based batch process with changing energy and media levels depending on the Process Operations and the stochastic state change-based energy and media levels of the units in the packaging/bottling area. The use case represents the brewhouse and a refillable glass beverage bottling plant and thus provides a good example of a beverage industry operation. The method is not limited in terms of the number or type of process cells. Another special feature is the integration of specific production schedules. This integration allows the realistic simulation of the real production and thus extends the scope for experimental investigations by adapting them. As a result, the overall course of the electrical and thermal energy for the use case is presented. Only the holistic view of a production operation allows the investigation of the influence on the entire system. This is essential especially for the avoidance of load peaks, for design planning of supply facilities, for the generation and use of recuperative energies and finally for the increase in energy and media efficiency by experimental investigations based on numerous influencing factors.

10. Conclusions

An approach for the modeling and simulation of batch-oriented operation with regard to energy and media requirements of plants of the beverage industry was presented. By using a previously presented modeling solution and by the development of a semi-automatic parameter determination tool, a model of a brewhouse can be created. In order to obtain a reliable database for the determination of the simulation parameters on the one hand and for the acquisition of validation data on the other hand, extensive measurement campaigns regarding brewhouse electrical and thermal energy demand were carried out. By using a configuration file, a simulation model can be automatically generated in a simulation environment and successfully verified. Based on three time periods, the entire method was successfully validated. Very small deviations were achieved throughout for the total and recipe-specific thermal and electrical energy consumption values. It can be concluded that the simulation method is very well suited to depicting and predicting the energy and media consumption behavior of process plants in the beverage industry in detail. The number of Process Operations within Process Stages influences accuracy immensely, which indicates a potential for improvement in the definition of these operations. This can be done by automated detection of the consumption-relevant Process Operations. In addition, the database plays an essential role for the accuracy of the energy and media consumption quantities within the time periods. Although an extensive database could be created, further data is advantageous, especially for a recipe-specific consideration. The automated storage of consumption data would eliminate the need for time-consuming measurement campaigns, data preparation and manual linking with contextual information. In particular, the presented database structure in connection with the nomenclature of the Weihenstephan Standards [43] offer a good basis for an automated connection of a process control system. In addition to the direct specification of the respective consumptions of the processes by the respective plant manufacturer, numerous advantages would result, in particular with regard to the design planning of the supply plants and the subsequent examination of optimization measures.

The claim to create a user-friendly method that can be used without specific previous knowledge or expert know-how in order to enable SMEs above all to increase their energy and media efficiency is guaranteed with the tools for automatic parameter determination, simulation evaluation and by the modeling solution including automatic simulation model generation. In particular, the modeling solution has been described and validated in detail [29].

The use case for simultaneous simulation of batch-oriented and discrete production mode in the brewery forms the overall picture from the previous work on the model for mapping holistic production systems of the beverage industry. This includes the implementation of the metamodel in a modeling editor [29] and automatic model generation and the simulation of the discrete packaging/filling area of beverage plants [16]. Furthermore, their specific recipes or articles can be mapped and simulated in a model with the inclusion of a production plan, which ensures a realistic simulation over even a longer period of time.

- The following scenarios for real use cases can be set up for which we believe the entire method is capable of solving: Prediction of realistic energy and media consumption of plants and machines.
  - For the correct design of utilities, since usually no or only very inaccurate information about the real consumption is available.
  - To detect unnecessary consumption, e.g., during downtimes and to apply consumption-oriented control.
  - To identify load peaks in certain time intervals to reduce and shift them in order to avoid overruns in the averaged power interval.
- Estimation and quantification of investments and their impact on the overall system.
  - Modernization of entire areas and individual units.
  - Capacity increases including any necessary adjustments to the supply structure.
  - Use of alternative sustainable energy generation systems (e.g., CHP plants, photovoltaic systems, etc.).
  - Use of energy and heat storage systems.
- Use of recuperative energies as well as waste heat in the entire production system.
- Adaptation of production plans for optimal energy and media utilization.
- Influence of factors and key figures (OEE, availability, etc.) on energy and media consumption to determine the optimal sustainable operation of the plants.

All application cases can contribute to more efficient and thus more sustainable production with the advantage that ongoing production is not affected or has to be interrupted. In addition, the entire method, through strict adherence to and implementation of ANSI/ISA 88 [39] structuring, shows potential transferability to other industries, such as the food, biopharmaceutical and chemical industries.

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Appendix A

Table A1. Overview of the simulation-relevant parameters of the “Pilsner” recipe.

Process Stage	**Process Operation**	**Duration**		**Electrical Energy Demand [kWh]**		**Thermal Energy Demand [kJ]**	
		MW	**95% KI**	**MW**	**95% KI**	**MW**	**95% KI**
Milling	Milling	5932	181.585	5.744	0.200	-	-x
Mashing	Mashing in	1663	56.100	22.334	1.050	-	-
	Heating up 1	61	6.303	0.0181	0.047 with a summed mean value of 1.457	63,242.47	7275.96
	Resting 1	1474	2.451	0.437		-	-
	Heating up 2	71	9.201	0.021		71,164.83	3455.64
	Resting 2	273	5.158	0.081		-	-
	Heating up 3	185	34.982	0.055		138,320.35	4138.56
	Resting 3	238	19.993	0.071		-	-
	Heating up 4	247	41.998	0.073		180,228.15	2328.48
	Resting 4	1935	10.747	0.574		-	-
	Heating up 5	302	38.145	0.090		134,430.97	1939.32
	Resting 5	125	0.350	0.037		-	-
	Final mash pumping	656	6.429	0.294	0.001	-	-
Lautering	Trub wort pumping	429	123.694	0.07	0.070	-	-
	Resting	223	8.326	-	-	-	-
	Lautering	5566	51.070	2.20	0.220	-	-
	Remove spent grains	661	7.841	0.44	0.450	-	-
Wort storage	Wort storage	32	1.469	-	-	-	-
Lauter wort heating	Lauter wort heating	1877	54.028	4.780	0.138	923,352.70	32,161.68
Keeping heat	Resting 1	80	1.001	0.003	0.003 with a summed mean value of 0.186	-	-
	Heating up 1	324	23.917	0.020		285,960.00	34,153.56
	Resting 2	2022	326.276	0.103		-	-
	Heating up 2	306	12.938	0.016		29,480.00	3773.16
	Resting 3	1279	374.267	0.044		-	-
	Casting	983	7.677	0.295	0.297	-	-
Sedimentation	Sedimenting	1230	64.335	-	-	-	-
Vaporization and Cooling	Vaporization & Cooling	3774	24.021	36.983	0.403	−2,930,540.80	42,980.04
	Rinsing	650	34.496	2.294	0.033	−298,660.00	3594.93

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3 Discussion

In this thesis, the approaches available in the literature for increasing the energy and media efficiency of production systems in the beverage industry were first examined, categorized, critically discussed and the resulting scientific gaps were identified. In addition, the barriers existing for SMEs with regard to increasing energy and media efficiency were named and the consumption structures as well as the main consumers in the brewery, as an example for the beverage industry, were uncovered. A metamodel based on four modeling pillars (physical, process, article/recipe, and production plan model) for generic, context-free, and holistic mapping of production systems is presented. The metamodel is implemented in a user-friendly modeling solution, which allows fast and easy modeling without prequalification of the user. As a result, a configuration file is presented and the approach is validated with respect to its suitability and usability. The configuration file represents the starting point for the further application of the method in the two differently operating production areas of the brewery. Based on this, the automatic generation of simulation models in a simulation environment, which was extended by the hybrid simulation considering a production plan, is developed and presented. The development of a standardized and generic data structure enables the storage of the measured real data as well as the simulation result data. Based on this, simulation parameters can be determined in a standardized way with the help of a defined procedure, implemented in software tools, and simulation runs can be evaluated. In the two production areas of the brewery, the batch area as well as the packaging and bottling area, an extensive and detailed validation with real data takes place and use cases show the application and suitability of the method. As a final result and as a way for enterprises in the beverage industry to achieve efficient and sustainable production, the hybrid simulation of a holistic production system is presented.

This thesis consists of four publications in logical and consecutive order, which step by step cover the whole approach of modeling and simulation of production systems of the beverage industry regarding energy and media demand. Starting from a literature work on the development of a metamodeling approach and its implementation, the development of the automatic simulation model generation as well as a hybrid simulation solution is presented and a detailed validation as well as application of the method based on real data are performed. According to the scientific questions defined in chapter 1.4, the results of this thesis are comprehensively discussed, summarized and reflected against the existing literature in the following sections.

3.1 SQ1: Generic metamodel for the modeling of complex hybrid production systems

The development of the presented metamodeling approach for the mapping of holistic and hybrid production systems of the beverage industry is divided into three stages and thus represents the basis for the entire methodology for modeling and simulation. So far, no metamodeling approach has been described in the scientific literature and modeling usually takes place only specifically for concrete use cases.

First of all, the metamodel, which is modeled in the unified language UML, has to be mentioned. Due to the clear graphical notation, the definition of the individual modeling columns, which were subdivided context-free according to the ANSI/ISA-88 standard [53] into plants, processes, recipes/articles as well as production plan, is clearly described. Thus, existing approaches [51, 63] for subdivision are adopted, combined, extended by the recipe/article as well as production plan model and extended to both production areas within the beverage industry. The hierarchical subdivision thus means maximum flexibility in horizontal and vertical granularity within the individual metamodel domains, since not only the depth of detail but also the scope of a model of a production system can be varied. The deepest modeling level of the metamodel is described as the “unit” level with respect to the physical model and as the “process operation” level in the process model. This level of granularity allows the mapping of detailed consumption patterns as well as peak loads. A higher level of detail would provide more accurate results, but requires a correspondingly greater effort of parameterization. Strict adherence to and implementation of ANSI/ISA-88 allows for transferability to other batch-oriented and discrete production systems such as those in the food, biopharmaceutical, and chemical industries. The description of the metamodel in UML also offers the advantage of suitability for Model-Driven Software Development (MDSD) approaches and can thus contribute to the development of modeling software.

The second stage is thus described by the transformation of the UML model into an XSD file. The terms and relationships stored in the graphical notation of UML can be made visible textually in other description types. Thus, the XSD defines all elements, attributes as well as data types and represents the structure of the UML class diagram.

The generic XSD serves thus as instance for the third stage, the XML configuration file, since it defines it and can be used for validation. The XML file is particularly characterized by its suitability for the exchange of data content, such as between the developed modeling solution and simulation environment used in this thesis.

Furthermore, the metamodel has the advantage that the system boundaries are defined and the information and parameters required for modeling or simulation emerge from the approach. This has not been described in the scientific literature so far and is therefore an essential contribution for the model development regarding the prognosis of the energy and media demand. Especially the data basis as well as the simulation parameter determination represent the main challenges here. In most cases, as numerous publications in this field show, the data basis is insufficient, which makes it difficult to determine statistically reliable parameters.

Ten different use cases from the publications II, III and IV, which are characterized by different plants in different areas, the plant configuration and composition as well as by different processes, recipes and articles within varying production schedules, clearly show that the developed metamodel is suitable for the entire method. The energy and media consumption behavior can be mapped and predicted realistically and simulation experiments regarding numerous factors could be performed.

3.2 SQ2: Implementation of the metamodel in a software to enable accessibility to the method

In the context of simulation studies, especially the modeling of the respective system to be examined takes up a large part of the time and specific know-how is usually required. Hence, a suitable solution, which implements the presented metamodel completely and with all its facets, is required. Therefore, the metamodeling approach has been fully implemented in a platform-independent software solution with the aim of creating models quickly, easily and at low cost. This is the prerequisite for a broad application of the method, which in turn can lead to a larger knowledge base and possible further open scientific questions. A strict implementation of the metamodel takes place through the context-free, hierarchical modeling columns, enabling generic and hybrid modeling. The individual modeling columns were thereby implemented considering already available works in modeling. Thus, the graphical modeling of the plant and the process model is based on the MES Modeling Language MES-ML [67, 68]. The physical modeling is done with the help of already predefined components, which are stored in a building block library. The elements are placed on a surface and linked with one another. Equivalently the hierarchical modeling of the processes takes place after ANSI/ISA-88 [53]. Since in this case MES-ML is based on BPMN, the modeling is clearly specified and unambiguously defined. The implementation of predefined process operations also standardizes and simplifies the modeling. The modeling of recipes and articles as well as the production plan result from the plant and process model. This further simplifies the modeling and no specific knowledge regarding simulation is required in this context. In this respect, the presented approach differs strongly from the complex solutions described in the literature, which are based, for example, on reference networks [93] or mathematical formulations [51]. The usability aspect of the modeling editor was addressed by specific implementations and functions. These implementations are discussed in Chapter 3.3 in context with the overall method.

The correct functioning of the modeling editor could be ensured through the ongoing verification by means of the already described XSD as well as a systematic test and the application of use cases. The systematic test included the factors "comprehensibility", "simplicity", "completeness" and "sustainability", which were consistently rated with at least "good" by the test persons. The results of the scientific survey on the application of the method were again implemented in the improvement of the solution and reviewed again. Thus, this question can be answered that the modeling solution is well comprehensible and easy to use. In addition, all relevant areas are covered and the editor shows potential for use in other industry sectors, which also corresponds to the objective of the metamodel. Although the modeling editor is tested in Publication II on the basis of use cases, the main application takes place in Publication III and IV on the basis of real plants with extensive databases.

3.3 SQ3: Development of a data structure, determination of simulation parameters and usability of the approach

To meet the requirement of developing a user-friendly method for predicting energy and media demand without requiring any specific prior knowledge or expert know-how on the part of the user, numerous implementations, tools and aids were created along the entire methodology. This should enable SMEs in particular to increase their energy and media efficiency with minimal effort and enable broad access to the method. Nevertheless, these developments can serve the entire industry as an aid as well as a template for further applications. So far, such a holistic method with regard to these requirements is not described in the scientific literature or commercially available.

As a first point, the development of the generic and extensible data format for the storage of measured raw data as well as simulation result data plays an essential role. Hereby it is possible to store all data of a production plant structured and divided into units, data points as well as into interval and time data. The data points are defined according to the Weihenstephan Standards (WS), which are available for the batch-oriented area of the brewery [95] as well as for the packaging and filling area [65]. This can mean enormous potential for a possible further development of the method (see chapter 3.6). The extension of the data structure by a production plan table implies maximum flexibility with regard to the determination of simulation parameters, which is done on the basis of the structure with the help of software tools. The generic parameter determination tools described in Publication III & IV were both developed in MATLAB AppDesigner [96]. These tools adapt to the respective database to be investigated and can determine simulation parameters with regard to various factors, such as recipe, article or also container type, fully automatically, in the discrete area, or semi-automatically in the batch area. This also enables comparability of the parameters and opens up further optimization potential. In addition to the parameters for describing the energy and media consumption behavior, the parameters for describing the failure behavior of the individual units are also determined in the discrete area. Due to the size of the database and the consistently low confidence intervals of all parameters presented in both publications, the values can be assumed to be reliable. The time required for parameter determination was demonstrably reduced considerably in both cases. This also applies to the creation of the models using the presented modeling editor.

The third point to be mentioned here are the numerous help functions that were implemented in the course of the development of the modeling solution. Thus, in addition to an extensive help menu with detailed step-by-step explanations, a function is also available for automatic checking with regard to the validity and thus the simulatability of the model against the XSD file. Furthermore, the predefined building blocks for modeling within the libraries, also through their graphical symbols, are intended to reduce complexity, thus overcoming the barrier of required expert know-how and making the method accessible to SMEs. In order to reduce the parameterization effort of extensive models and thus to achieve faster modeling, numerous automatic parameterizations have been implemented in the editor on the basis of the specification of a small amount of information, such as through the specification of the packing ratios or also the automatic calculation of the buffer capacity for different bundles. All three points could be tested and verified by the systematic test as well as by the application of the method especially in Publication III & IV and therefore contribute to a simple and fast model generation.

3.4 SQ4: Development of automatic simulation model generation

Based on the XML configuration file of the modeling editor, an automatic generation of simulation models for production plants of the beverage industry is described for the first time. Since the XSD schema describes and defines XML files, all models resulting from the approach follow this specification. As a result, on the basis of the XSD file, the connection to any simulation environment can be made once and the automatic generation of the simulation models on the basis of the XML files can be ensured. As a use-case, the simulation environment developed and used in this work was extended by the corresponding function. Therefore, any simulation environment, which masters the hybrid simulation of both production areas, can be adapted to the XSD file and thus be extended by the automatic simulation model generation. As an example, the described simulation of the packaging area in the software Plant Simulation could be mentioned [83]. The simulation model generation is based on the reproduction of the structures created in the modeling editor depending on the process cell as well as in the initialization of the elements with the corresponding parameters. This is based on the use of a uniform coordinate system as well as the definition of generalized elements that cover the functions required for mapping hybrid production systems. For this reason, the elements differ fundamentally in their behavior with regard to their operating mode, energy and media consumption, but also with regard to special functions that reflect the particularities of the complex units within the beverage industry. Another special feature is the continuous change of the simulation parameters by different recipes or articles during the simulation runtime due to the mapping of the production plan.

The approach has been intensively verified manually, validated and tested on use cases in Publication II. In Publication III a detailed application for the packaging or filling area takes place, whereas in Publication IV the application area is the batch area of the brewery. In this work, automatic simulation model generation for a holistic and hybrid production system also takes place for the first time. For this purpose, the brewhouse is simultaneously generated and finally simulated with a beverage bottling plant in one single model. The successful validations show that automatic generation of simulation models is the tool of choice for the creation of reliable and fast simulation models.

3.5 SQ5: Development of holistic hybrid simulation

The holistic and hybrid simulation of energy and media demand in the beverage industry using the brewery as an example represents the final objective of this dissertation. Through numerous steps, such as the development of a modeling approach in Publication II, the automatic simulation model generation and simulation in the packaging area (Publication III) as well as in the batch area (Publication IV), this goal could be achieved. Both areas were validated individually (Publication III & IV). In the packaging area the holistic simulation of all energy and media types for beverage filling, based on an extensive database, was described for the first time. It could be shown that the description of the energy and media consumption behavior purely based on the operating state shows similar results in the validation as the work with a further time-dependent consideration within the operating states [64]. Furthermore, the simulation of the brewery's batch area for thermal and electrical energy demand including a production schedule represents a novelty. Previous approaches are mostly limited to the thermal energy consumption in a restricted time period and usually no validation is considered in detail. By considering a production plan, the energetic consideration is extended by the off-period, i.e. non-production periods, e.g. on a weekend, and the related consumption level. In both subareas, the electrical and thermal energy consumption values of the real and simulated data are within a total deviation of about two percent. Outliers could be explained with the help of additional information or attributed to an insufficient database.

As the use case in Publication IV shows, the hybrid simulation makes it possible for the first time to take a holistic view of production operations in the beverage industry, such as breweries, which are characterized by differently operating subareas and the associated differences in consumption behavior. This enables the interdependencies of the brewery's complex production to be analyzed and optimization potential to be identified in a holistic approach. This is essential, especially with regard to design planning, the use of recuperative energy or also in the testing of optimization measures or the quantification of investments.

4 Final remarks and outlook

This thesis presents a holistic and hybrid approach for modeling and forecasting the energy and media demand of production systems in the beverage industry using the example of a brewery. It could be shown that a metamodel-based modeling approach in combination with an automatic model generation is able to create an executable simulation model and to perform both validation and simulation experiments. The claim of a fast, simple and user-friendly overall method that meets the requirements of SMEs, overcomes their barriers to energy efficiency and opens the method for a broad application, was proven on the basis of a systematic test in the course of a survey. The presented approach can already find practical application in the field of energy efficiency optimization in the beverage industry, but still offers further possibilities for improvement and further development.

Thus, it is conceivable to extend the method with regard to the following factors. On the one hand, the integration of energy and media sources as well as sinks would add another dimension to the simulation method and allow especially investigations regarding the generation and reuse of recuperative energy in a much more detailed way. On the other hand, the integration of other simulation methods, such as Pinch analysis, is also conceivable in this course.

The application of the method opens up the possibility of extending it to other areas within the beverage industry that have not been considered so far, as well as to other branches of industry. Thus, the method could be used in similarly operating production facilities, such as in the food and pharmaceutical industries. The mapping of further areas, such as the supply facilities, makes it possible to investigate the suitability of alternative energy sources such as photovoltaic systems or combined heat and power plants. In combination with short-term forecasts of the total energy demand, direct control of production operations to prevent peak loads, by shutting down facilities or via buffering using batteries, would also be conceivable.

Since reliable simulation studies are heavily dependent on the scope and quality of the raw data obtained from the production process and no holistic concept for collecting measurement data has been described to date, there is an urgent need for research. For the area of beverage filling and packaging, an approach for determining consumption data based on operating conditions has already been described [97]. Nevertheless, a concept for recording energy and media consumption in the area of batch-oriented production, for which this thesis can be an initial basis, is required. Furthermore, a comprehensive, standardized measuring concept with the exact description of the measuring points would be advantageous in order to obtain a sound and comparable data basis in any case.

To ensure a reliable and standardized database, the following concept for automatic data acquisition can be outlined. Thus, the WS [65] enable far-reaching possibilities in the application. On the one hand, numerous standardized data points are available for beverage filling and packaging plants as well as for brewing and beverage plants with regard to energy and media demand and operating behavior. In combination with an appropriate measurement concept, the data could be collected uniformly and stored, for example, in the data structure presented. On the other hand, this provides another opportunity which could further simplify the entire method. It is conceivable, that higher-level IT systems, such as a Process Control System (PCS) or MES, or even the units themselves can offer the data required for a simulation in the presented data structure according to the WS. In connection with Internet of Things (IoT)-capable machines in the course of Industry 4.0, the data could also be recorded directly and the entire phase of time-consuming measurement data acquisition could become obsolete.

This opens up a further possibility for simplifying the method presented, since a model structure could be automatically created on the basis of this data acquisition and the corresponding simulation parameters could be determined directly with the aid of the intelligent machines or with the parameter determination tools presented. Thus, it is conceivable that also the model generation phase, which still takes a large part of the time of simulation studies, can be automated and the simulation models are automatically generated based on the data structure.

5 References

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