Dissertation

Modeling of Energy Systems for Complex Simulations

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Ao.Univ.Prof. Dipl.-Ing. Dr.techn. Karl PONWEISER
Institut für Energietechnik und Thermodynamik/E302

eingereicht an der Technischen Universität Wien
Fakultät für Maschinenwesen und Betriebswissenschaften

von

Ines Leobner
0126159

Wien, am _____________ ________________________

Abstract

The thesis at hand presents a framework to design complex models and simulations of systems focusing on energy performance. It contributes to the research question, how to design and operate complex on-site energy systems of final energy consumers in the most sustainable way. A state of the art approach to answer this research question is to perform an energy system or building performance simulation, observing the energy system and the building. However, the operating efficiency of an energy system is also highly dependent on the consumers it supplies and vice versa. Therefore, in order to improve the allover system performance a profound knowledge of the consumer structure and behavior is required. Moreover, economic boundaries, competitiveness and the challenges of the changing energy market must be taken into consideration as well.

In order to predict the performance of a system based on simulation and derive recommendations for the design and operation of an energy system, all these influences must be integrated into the simulation. This can be accomplished either by integrating all the observed elements of the system into a comprehensive model executed in one single simulation environment or connecting several simulation environments to a so called cooperative simulation or co-simulation. Both ways have their advantages and disadvantages and the decision which one to pursue must be weighed carefully. Usually the undertaking of assembling, executing and interpreting such a complex, hybrid simulation involves experts from a number of different disciplines, collaborating on the modeling and simulation task. This thesis aims to provide a framework, which guides through this process.

Based on a comprehensive review of the state of the art on modeling and simulation theory, building performance and energy system simulation and simulation of complex systems and cooperative simulation a reference model for modeling of complex energy systems is presented. After the reference model an according approach for the design of the energy system model itself, considering the specific challenges rising from the embedding in a complex simulation environment, is discussed.

The chosen approach was developed in a hands-on approach in the course of two interdisciplinary research projects, which are presented as application examples. One project deals with the development of a software planning tool for optimization of the energy performance of manufacturing companies and the other project aims at the implementation of a model predictive controller in an office building in order to minimize the heating and cooling energy demand. Hence, it raises the additional challenge of a real-time application. To conclude the limitations and further development potentials of the proposed approach will be discussed concerning another application example in the field of the manufacturing industry, with a slightly different focus and therefore other requirements to the models.

The suggested approach is employable for different types of problems and application fields, such as industrial plants, public buildings and community facilities, office buildings, etc. Furthermore, different scopes with respect to the mode of operation of the simulation exist. The most obvious is as a planning support tool for a new building or facility. But in recent years, along with rapid developments in computer hardware, the implementation of simulations into daily operational planning routines and even controls become more and more realistic or even customary.

Kurzfassung

Die vorliegende Arbeit präsentiert einen Bezugsrahmen für das Design komplexer Modelle und Simulationen von Systemen mit Fokus auf das energetische Verhalten. Sie trägt zur Lösung der Forschungsfrage, wie komplexe Endenergienutzer Systeme nachhaltig ausgelegt und betrieben werden können, bei. Der Zugang zu dieser Forschungsfrage nach Stand der Technik ist, eine Energiesystem oder Gebäudesimulation durchzuführen, welche das Energiesystem und Gebäude abbildet. Die Effizienz eines Energiesystems im Betrieb ist jedoch auch stark von den Nutzern die es versorgt abhängig und vice versa. Daher ist, um die Effizienz des Gesamtsystems zu erhöhen, ein tiefgreifendes Verständnis der Nutzerstruktur und des Verhaltens notwendig. Außerdem müssen ökonomische Randbedingungen, Wettbewerbsfähigkeit und die Herausforderungen des sich verändernden Energiemarktes ebenfalls in die Betrachtung mit einbezogen werden.

Um das Verhalten eines Systems auf Basis einer Simulation vorhersagen zu können und Empfehlungen für Auslegung und Betrieb des Energiesystems ableiten zu können, müssen alle diese Einflüsse in die Simulation mit einbezogen werden. Das kann durch die Integration aller Elemente in ein umfassendes Modell, das in einer Simulationsumgebung ausgeführt wird, oder durch die Kopplung mehrerer Simulationsumgebungen in eine sogenannte Co-Simulation realisiert werden. Beide Varianten haben Vor- und Nachteile, die sorgfältig abgewogen werden müssen. Üblicherweise involviert das Zusammenstellen, Ausführen und Interpretieren solch einer komplexen, hybriden Simulation Experten mehrerer unterschiedlicher Disziplinen, die an der Modellierungs- und Simulationsaufgabe zusammenarbeiten. Diese Arbeit stellt einen Bezugsrahmen bereit, der durch diesen Prozess führt.

Basierend auf einer umfassenden Analyse des Standes der Technik in Bezug auf Modellierungs- und Simulationstheorie, Gebäude- und Energiesystemsimulation und Simulation komplexer Systeme, sowie Co-Simulation, wird ein Referenzmodell für die Modellierung komplexe Energiesysteme vorgeschlagen. Danach wird ein abgestimmter Zugang zum Design von Energiesystemmodellen an sich präsentiert, welcher auf die spezifischen Herausforderungen, die aus der Einbettung in komplexe Simulationen resultieren, Bezug nimmt.

Die ausgewählte Herangehensweise wurde durch praktische Durchführung im Rahmen von zwei interdisziplinären Forschungsprojekten entwickelt, welche als Anwendungsbeispiele beschrieben werden. Ein Projekt beschäftigt sich mit der Entwicklung eines Planungswerkzeugs für die Optimierung der Energieeffizienz in Fertigungsbetrieben und das andere Projekt zielt auf die Implementierung eines modellprädiktiven Reglers in einem Bürogebäude ab, um den Heiz- und Kühlenergiebedarf zu minimieren. Es stellt daher die zusätzliche Herausforderung der Echt-Zeit Anwendung auf. Im Abschluss werden die Grenzen und Weiterentwicklungsmöglichkeiten des vorgeschlagenen Ansatzes anhand eines anderen Anwendungsbeispiels im Bereich der industriellen Produktion, bei dem sich aus einem veränderten Fokus andere Modellanforderungen ergeben, diskutiert.

Die vorgeschlagene Herangehensweise ist für unterschiedliche Probleme und Anwendungsfelder anwendbar, wie z.B. für industrielle Anlagen, öffentliche und Bürogebäude, etc. Darüber hinaus gibt es verschiedene Möglichkeiten für die Betriebsart der Simulation. Die offensichtlichste ist als Planungsunterstützung für Neubauten, aber in den letzten Jahren, mit der rasanten Entwicklung der Computer Hardware, wurde die Implementierung von Simulationen in tägliche operative Planungsroutinen und sogar Regelungen immer realistischer und üblicher.

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List of Publications

Parts of this thesis have already been contributed by the author to the following publications:

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Popper, N., I. Hafner, M. Rössler, F. Preyser, B. Heinzl, P. Smolek, and I. Leobner, "A General Concept for Description of Production Plants with a Concept of Cubes," *SNE - Simul. Notes Eur.*, vol. 24, no. 2, pp. 105–114, 2015.

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Ferhatbegovic, T., S. Hauer, I. Leobner, K. Ponweiser, A. Schirrer, and M. Kozek, "Thermal building modeling and simulation for automated load shifting purposes in the non-residential building sector," in *eWork and eBusiness in Architecture, Engineering and Construction: ECPPM 2014*, 2014, pp. 511–516.

Orehounig, K., A. Mahdavi, I. Leobner, and K. Ponweiser, "System analysis and coupled modeling: toward integrated performance assessment of industrial facilities," in *eWork and eBusiness in Architecture, Engineering and Construction: ECPPM 2012*, 2012, pp. 3–8.

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Heinzl, B., M. Rossler, N. Popper, I. Leobner, K. Ponweiser, W. Kastner, F. Dur, F. Bleicher, and F. Breitenecker, "Interdisciplinary Strategies for Simulation-Based Optimization of Energy Efficiency in Production Facilities," in *2013 UKSim 15th International Conference on Computer Modelling and Simulation*, 2013, pp. 304–309.

Heinzl, B., W. Kastner, M. Rößler, F. Bleicher, F. Dür, I. Kovacic, I. Leobner, and N. Popper, "Interdisziplinäre Optimierung der Energieeffizienz in Fertigungsbetrieben mittels Co -Simulation Co-Simulation," in *ASIM-Workshop der STS/GMMS 2014*, 2014, pp. 1–4.

Dür, F., T. Flatz, I. Kovacic, L. Waltenbereger, D. Wiegand, S. Emrich, I. Leobner, T. Bednar, K. Eder, W. Kastner, B. Heinzl, and K. Kiesel, "Endbericht INFO - Interdisziplinäre Forschung zur Energieoptimierung in Fertigungsbetrieben," Vienna, 2013.

Ferhatbegovic, T., W. Gawlik, R. Haas, M. Hartl, S. Hauer, M. Heimberger, S. Henein, A. Hiesl, P. Jasek, R. Klug, B. Kodre, M. Kozek, F. Kupzog, M. Leitner, I. Leobner, K. Ponweiser, S. Schidler, A. Schirrer, J. Stockinger, H. Taus, M. Volcic, and G. Zucker, "Endbericht SmartCityGrid:CoOpt," Vienna, 2015.

Contents

1. Introduction

1.1. Motivation

Since the invention of the steam-engine and the subsequent development of generators, turbines, combustion engines enabled humanity to supply useable energy at practically every time and place an accelerated technological progress and substantial growth of wealth has taken place. These advances in turn lead to an augmented energy demand which has been almost exponentially growing since the industrial revolution and continues to do so until today. Even in industrial countries with a relatively low growth of population the final energy demand is still increasing.

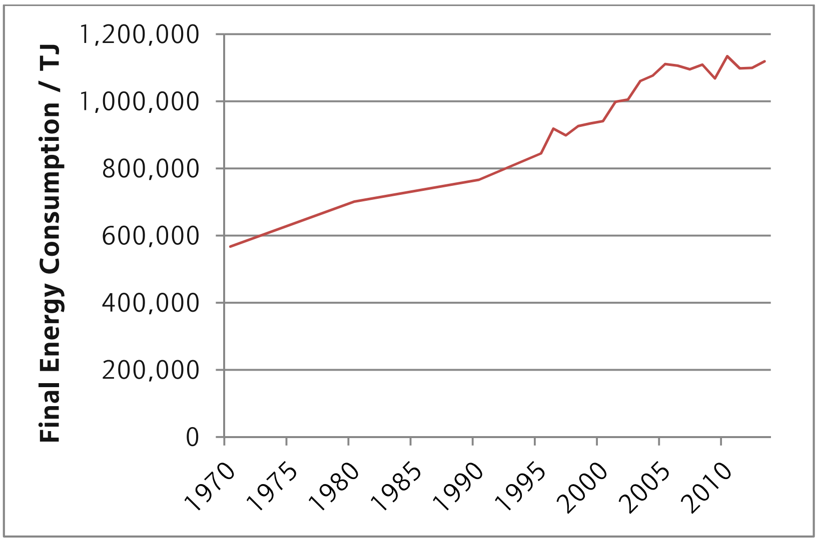

Figure 1: Development of final energy consumption in Austria 1970 - 2013, data source: [1] Gesamtenergiebilanz Österreich (1970 - 2013)

Also in terms of energy sources and use a major shift has taken place. In pre-industrialized societies agriculture was the main consumer of energy which was almost exclusively gained from renewable sources. [2, p. 5] Nowadays industrialized countries show a completely different supply and demand structure, as can be seen in Figure 2.

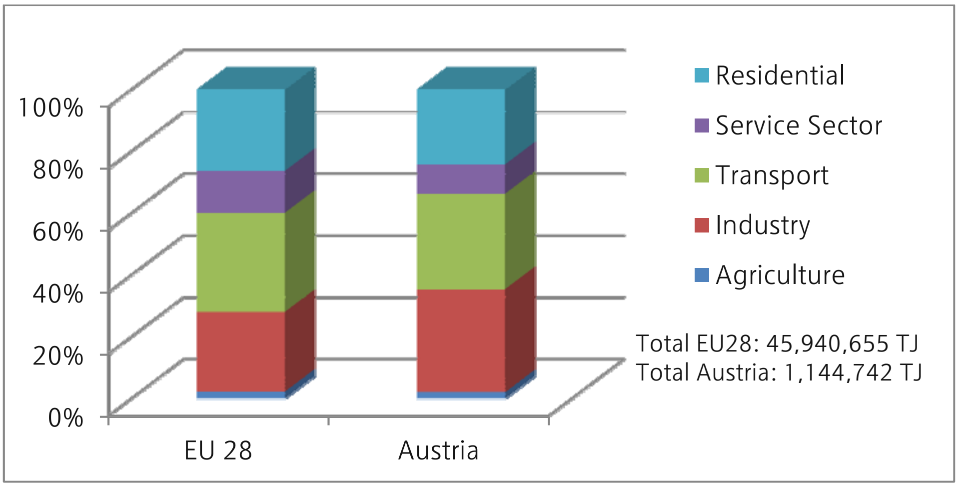

Figure 2: Final Energy consumption EU 28 and Austria by sector in 2012, data source: [3] Energy balance sheets 2011 - 2012 (2014 edition)

As a result of these developments it finally had to be acknowledged in the late 20th century that the lavish handling of resources maintained in the last decades also causes severe damages to the environment and the planet. The globally most threatening consequence is, of course, the climate change, which raises a number of challenges for our society in order to preserve our planet for future generations.

Policy makers around the world pursue different strategies in order to successfully combat climate change and preserve our planet for future generations. The President of the United States has committed the country in his Climate Action Plan [4] to reduce the U.S. greenhouse gas emissions by 17% below the levels of 2005 until 2020. China's 12th Five-Year Plan establishes a set of three goals, similar to the European Union. A 16% reductions in energy intensity (energy consumption per unit of GDP), a 17% reduction in carbon intensity and an increase of non-fossil energy to 11.4% are targeted until 2015 [5]. The European Union follows a longer term strategy consisting of the "2020 energy and climate package" [6], a "Policy framework for climate and energy in the period from 2020 to 2030" [7] and the "Energy roadmap 2050" [8], which establish step-by-step goals until reaching reducing the greenhouse gas emissions to 80-95% below the level of 1990 in 2050 [8, p. 2].

The 2020 energy and climate package, currently under action, establishes the well known 20-20-20 targets:

- 20% reduction in greenhouse gas emissions compared to the level of 1990
- 20% of EU energy consumption produced by renewables
- 20% improvement in energy efficiency.

In order to achieve the energy efficiency target the "Energy efficiency plan" [9] emphasizes the need for action and outlines the strategic plan to achieve the set goal:

> *Energy efficiency is at the heart of the EU's Europe 2020 Strategy for smart, sustainable and inclusive growth and of the transition to a resource efficient economy. Energy efficiency is one of the most cost effective ways to enhance security of energy supply, and to reduce emissions of greenhouse gases and other pollutants. In many ways, energy efficiency can be seen as Europe's biggest energy resource.* [9, p. 2]

The plan identifies a number of main action fields, among which the main energy consumers - buildings, industry and transport – are targeted. The implementation of the Energy efficiency plan again is driven by a legislation framework, containing among other statutes the Energy Efficiency Directive (2012/27/EU), the Energy Performance of Buildings Directive (2010/31/EU) or the Energy Labeling Directive (2010/30/EU). Despite all legislative effort to achieve the set target the path towards energy efficiency is a stony one. While the other two targets seem within reach, Eurostat's 2015 report on the 2020 targets states that the primary energy consumption, which serves as an indicator for energy efficiency, has been decreasing, however, that this development is most likely due to reduced economical activity in recent years [10, p. 95]. Therefore, there is a clear need for action, which has been recognized in the Union's research policy. According to the annex of the Regulation (EU) No. 1291/2013 [11], which establishes the "Horizon 2020" research framework program, one of the seven main societal challenges the research program is targeted towards, is secure, clean and efficient energy. As a line of activity within this focal area energy use takes a leading position:

> *Reducing energy consumption and carbon footprint by smart and sustainable use*

> *Activities shall focus on research and full-scale testing of new concepts, non-technological solutions, more efficient, socially acceptable and affordable technology components and systems with in-built intelligence, to allow real-time energy management for new and existing near-zero-emission, near-zero-energy and positive energy buildings, retrofitted buildings, cities and districts, renewable heating and cooling, highly efficient industries and mass take-up of energy efficiency and energy saving solutions and services by companies, individuals, communities and cities.* [11, p. 155]

As quoted above, the Horizon research framework sees in-built intelligence and real-time energy management as a future research challenge concerning responsible energy use. In order to design efficient systems and develop these intelligent steering tools, a profound understanding of the underlying physical or informational system and its behavior is mandatory.

1.2. Objectives

In this context one of the core research questions, to which this thesis contributes, is how to design and operate the often rather complex on-site energy systems of consumers in the most sustainable way.

A state of the art approach to answer this question is to perform an energy system or building performance simulation. However, the system simulation solutions, currently available on the market can only provide answers to a certain extent, because they usually limit the observed area to the energy system and the building. However, the operating efficiency of an energy system is also highly dependent on the consumers it supplies and vice versa. Therefore, in order to improve the allover system performance a profound knowledge of the consumer structure and behavior is required. Moreover, with the increasing integration of fluctuating renewable energy source and the resulting challenges to the balancing energy market, additional challenges for, especially larger, consumers arise. And last but not least economic boundaries and competitiveness must be taken into consideration as well. In order to predict the performance of a system based on a simulation and derive recommendations for the design and operation of an energy system all these influences must be integrated into a simulation. In order to accomplish this task two approaches for the technical implementation exist. Either all the observed elements of the system are integrated into a comprehensive model executed in one single simulation environment or connecting several simulation environments to a so called cooperative simulation or co-simulation. Both ways have their advantages and disadvantages and the decision which one to pursue must be weighed carefully. Usually the undertaking of assembling, executing and interpreting such a complex, hybrid simulation involves experts from a number of different disciplines, who need to develop a common knowledge base related to the discussed problem.

In order to address these challenges this thesis tries to develop a guideline and framework to design complex or hybrid simulations of systems focusing on energy performance related problems and an according approach for the energy system simulation itself.

1.3. Structure of the Thesis

From the above mentioned challenges derives the structure of the thesis.

As a starting point a comprehensive review of the state of the art is given, covering mainly the following topics:

- General aspects of modeling and simulation
- Modeling and simulation processes
- Theory of conceptual modeling and basics concepts of mathematical models
- Concepts and applications of building performance and energy system simulation and recent developments in research
- Theory and implementation of modeling and simulation of complex systems and cooperative simulation

Since the scientific work that led to this thesis is based on previous projects and was executed in interdisciplinary project teams, some other theses' examining related topics exist. They are discussed in more detail and their implication on the current work is surveyed.

In the next chapter the developed process for designing a reference model for simulation of complex energy systems is presented. The chosen approach was developed in a hands-on approach in the course of an interdisciplinary research project and retrospectively formalized using model development methodologies and tools.

After the reference model the energy system model itself is regarded in more detail. The specific challenges for the energy system model rising from the embedment in a complex simulation environment are discussed. Based upon these considerations a model structure for the overall energy system model to match the reference model is suggested. From there adequate formulations for the models of the most common energy system models are derived.

In order to illustrate the proposed approaches and prove its feasibility two application examples, developed in two interdisciplinary research projects with a different scope will be presented. One example deals with the development of a software planning tool for optimization of the energy performance of manufacturing companies and the other project aims at the implementation of a model predictive controller in an office building in order to minimize the heating and cooling energy demand. Hence, it raises the additional challenge of a real-time application.

To conclude the limitations and further development potentials of the proposed approach will be discussed concerning another applications example, with a slightly different focus and therefore different requirements to the models.

1.4. Context

The suggested approach is employable for different types of problems and application fields. Especially energy consumers with a complex supply and/or demand structure may profit of a hybrid simulation. This may include:

- Industrial plants
- Public buildings and community facilities
- Office Buildings
- Buildings for trade industry and services sector

Furthermore different scopes with respect to the mode of operation of the simulation exist. The most obvious is as a planning support tool for a new building or facility in order to compare the influence of different system configurations or parameters on the energy use or environmental impact. But in recent years, along with rapid developments in computer hardware, the implementation of simulations into daily operational planning routines and even controls became more and more realistic or even customary. This opens up another application field for complex simulations.

As mentioned before the approach proposed in this thesis has been developed and tested on two different scenarios. The first one was as a planning tool for manufacturing plants and the other one was as a part of a model predictive controller of the heating and cooling demand of an office building. Both simulations were developed in collaborative research projects funded by the Austrian government via means of the Climate and Energy Fund within the funding program "New Energies 2020".

Project INFO – Interdisciplinary Research towards Energy Optimization in Manufacturing Companies

The research project INFO [12] started in 2010 and was one of the first research projects to conduct a holistic investigation on energy use for manufacturing goods. The aim was to generate energy-efficient optimization of production facilities and halls. Initially the project was mainly geared towards the metal-cutting industry, but it turned out that major parts of the developed approach are more universally applicable. Motivation to initiate the project was on one hand the large share of the industrial sector of society's total energy consumption combined with the significant potentials for reduction that had been demonstrated in numerous case studies [13] and on the other hand the rising pressure on the industrial sector itself to take action. For decades the ultimate optimization goal of the industrial engineering sector had been the increase of productivity and decrease of costs. But due to additional demands, such as legislative pressure, consumer awareness and rising energy costs, energy efficiency had become an increasingly important topic in the manufacturing industry by then.

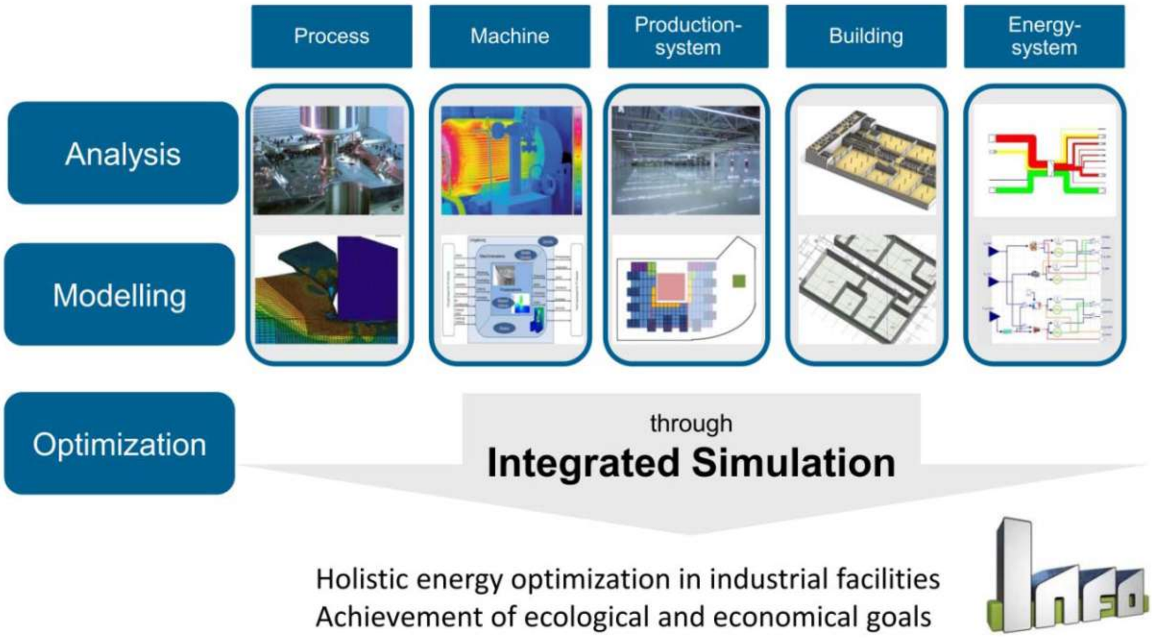

Figure 3: Optimization fields in a production plant as identified in project INFO

Some optimization approaches (e.g. use of sustainable materials, reduction of energy consumption, minimization of manufacturing costs, shortening the supply chain, reduction of resources, decrease of machine and tool wear or design of production facilities) were the subject of many research projects and were becoming state-of-the-art in the industry. The project built on these approaches and strived to create an interdisciplinary point of view on this field of research. The detailed examination of the optimization fields and their influences upon each other were considered crucial in order to achieve an overall optimum design of a production plant. In order to assess the energy flows and single out the interdependencies, goal of the project was to assemble an integrated simulation and conduct a case study about one of the project partner's production sites. To achieve this objective the system 'production plant' was intersected into optimization fields (see Figure 3), which were subsequently analyzed and modeled by the respective domain experts. But in order to advance from this state to an integrated simulation and visualize the additional benefits of a holistic approach a methodology for model coupling was required.

The integrated simulation was designed to be reused as a planning tool for manufacturing companies. Furthermore, as a final result, a roadmap to energy efficient production [14], targeted at industrial user groups, was edited from the project results.

Project SmartCityGrid:CoOpt – Coordinated Optimization of Renewables in Grid and Building in Planning and Operation

The project SmartCityGrid:CoOpt was established in 2012. Previous investigations of project partners had demonstrated that in an urbanized city district 100% coverage of the electrical energy demand by means of renewable but fluctuating energy sources over the year is in principle possible. However, due to temporal distribution of demand and supply and technical restrictions of the existing urban electric energy system the self coverage is limited [15]. Storage systems can only counteract this problem to a certain extent. So in order to reach a global optimum in the sense of direct utilization of renewable energy and energy efficiency, the overall electric distribution network in context with the supplied buildings must be considered. Therefore, SmartCityGrid:CoOpt tried to develop a global systemic energy management at the levels of the building and the distribution network.

The project set out to achieve this goal by an optimized use and integration of thermal and electrical storages and passive storage masses in buildings into the urban energy management. By exploiting load shifting potentials the locally produced renewable energy should be integrated optimally into the operation of the building and of the energy network. To realize this, a methodology for optimized control strategies, based on model-predictive controllers (MPC), was developed. In order to realize a global systemic optimization, hierarchical control concept, containing a building controller on the lower level and a grid controller, was developed. As a reference case for the building controller a real building was modeled and operated with the developed controller. Exact models and predictions, related to the development of demand, production, and consumption or weather related forecasts, were assemble with the actual predictive control algorithm into a simulation framework and later on into a hardware-in-the-loop application with the real building. The results were linked to the grid simulation and controller in order to achieve a holistic methodological approach, as well as strategies for an overall systemic, coordinated optimization. Quantification of the impacts on sustainability showed that an optimization by means of model predictive control is a substantial improvement compared to existing operation methods of buildings and distribution networks in cities and indicated which potentials for increased efficiency could be expected. The successful hardware-in-the-loop test could further on demonstrate that simulations are increasingly feasible for being used in real-time applications.

A more detailed description of the projects and the findings concerning the complex simulation process and the achieved energy savings can be found in Chapter 5 and 6. Furthermore, the findings of the project INFO led to the constitutive research question of applying the developed analysis and research methodologies not only to planning processes but also to operational steering of manufacturing plants. Also the development of a marketable product was a challenge at hand. Out of these ideas the project Balanced Manufacturing [16] originated in 2014. This follow-up project and the implications of the research discussed in this thesis on it are examined in Chapter 7.

2. State of the Art in Energy System Modeling and Simulation

In this chapter an overview of modeling and simulation (M&S) concepts in general and of M&S of energy systems and complex systems aligned to this thesis are given. General aspects and concepts of modeling and simulation will be discussed, with focus on their application for assessment of energy flows and systems. Common tools for modeling and simulation of energy systems and related domains will be reviewed and the state of the art in model coupling will be summarized. Furthermore, several works closely related to the topic of this thesis will be examined in more detail.

2.1. Simulation – System – Experiment – Model

In literature a number of different definitions for "simulation" can be found. The most universal definition is simply formulated as:

A simulation is an experiment performed on a model. [17, p. 6]

Other attempts to define a simulation also add in the factor time and a specification of the observed object:

A simulation is the imitation of the operation of a real-world process or system over time. [18, p. 3]

While in some cases the latter definition might be too limiting, it is, however, the most commonly assumed definition for the purposes of scientific investigations in the field of energy system and building performance analysis.

As for the system itself, again a multitude of different definitions exist. The briefest ones simply define it as a potential source for data [17, p. 4] or as an object or a collection of objects whose properties are the interest of study [19, p. 2]. Other authors go into more detail about the nature of systems. Most sources linked with the scientific domains of thermo- or hydrodynamics define a system mainly by its boundary, separating it from the environment [20, p. 15], [21, p. 4]. Other definitions of systems rely on the description of their interior composition, such as given by Popper in [22, p. 13]:

A collection of interacting or interdependent objects is called a system. The objects are the components of the system.

Both approaches for defining a system are in some way relevant for the task of simulation of complex energy systems. The boundary approach provides the necessary foundation for energy system models based on balances. On the other hand the understanding of systems as a number of interacting objects is essential for the handling of complex systems in modeling and simulation tasks.

Some sources, such as [23] demand that the system must show a dynamic behavior, in other words must change its behavior over time. This may lead to some confusion concerning the wording, because the term "dynamic" is used in a different sense in different domains. In the source mentioned above the term is used to generally characterize a system whose behavior shows changes over time. However, in the domain of thermodynamics and energy system modeling the term is usually attributed to a narrower definition characterizing properties of the system, as explained in more detail later.

A further characteristic of systems is that they possess inputs and outputs. Inputs are variables that influence the system from the environment. They may be controllable or act as a disturbance. Outputs are variables that are determined by the system behavior. They may have the ability to influence the environment or simply consist of data obtained from the system. This directly leads to the definition of the experiment, which is according to Cellier:

> *An experiment is the process of extracting data from a system by exerting it through its inputs*. [17, p. 4]

In some cases it may not be feasible to conduct the experiment directly with the system for different reasons. A non-comprehensive list of which is given in [17, p. 10]:

- The system is not available.
- The experiment is too dangerous.
- The experiment is too expensive.
- The time constants of the system are not compatible with the experimenter.
- Variables and/or parameters of the system are not accessible.
- Disturbances or second-order effects need to be suppressed.

If one or more of these cases apply another option to gain the desired information about the system, is to represent the decisive properties of the system in an alternative way:

> *A model of a system is anything an "experiment" can be applied to in order to answer questions about that system*. [19, p. 6]

Apart from the very rare case were a model is the exact reproduction of the original system (which may be desired for some experimental designs), this definition of a model implies that it is a somehow simplified version of the real system that only takes the determining features to answer the question at hand into account. This leads to the popular statement, quoted by Loper [24, p. 6], that *essentially all models are wrong and some models are useful*. Therefore, the abstractions and assumptions made in the modeling process must always be carefully weighed with regard to the intended experiment performed on the model. Conversely the reuse of models outside of their originally intended purpose may lead to doubtful results.

The given definitions of a model and a system also imply that the model again is a system, which can again be represented by a model of the model (meta-model), and so on and so forth. Since a model is a system it must possesses the same properties a system has i.e. consist of interdependent and interacting objects (see system definition above). This means that a component of a model is again a new model and valid for a subset of experiments the original model was valid for [17, p. 5], [19, p. 6].

Also nowadays models and simulation are commonly associated with an operation carried out with the help of a computer. It might be worth noting at this point that according to the definitions above models and simulation are understood in a much broader context and have existed significantly longer than computers. Physical models for static and dynamic experiments have been used throughout history e.g. architectural models or battle simulations with maps and figures representing armies. Also mental and verbal models can be useful tools to create a common understanding of a system. However, in computer simulation mathematical models are usually the tool of choice and as such represent a core concept of simulation and modeling. Therefore, the different types and properties of models will be described in more detail in Chapter 2.3.2.

2.2. Modeling and Simulation Process

The previous sections defined some of the basic concepts and components of modeling and simulation in general. This section will deal with the process of deriving a model from a problem in general and implementing an executable simulation. A number of suggestions for the process design are available from the literature for simulation studies of varying size and complexity [18, p. 15], [25]–[30]. For reference the approaches of Banks, Sargent and Balci will be discussed in more detail, since they provide the main basis for the considerations in the following chapters.

Banks provides a quite straight forward approach for simulation studies as decision making support tools consisting of twelve steps, as summarized in Figure 4 [18, p. 15] and below.

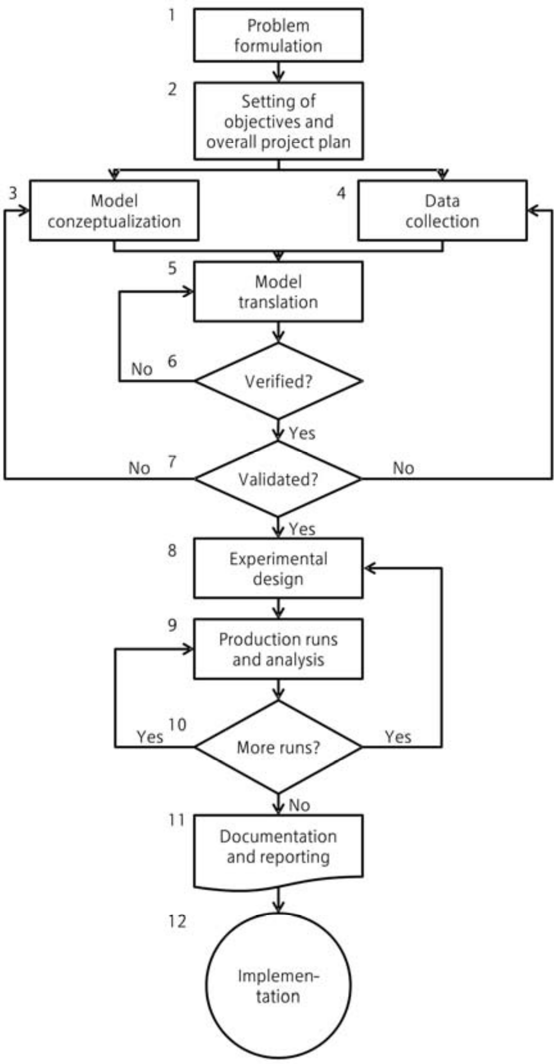

Figure 4: Steps of a simulation study according to Banks[18, p. 16]

1. Problem formulation. The problem must be described clearly and it must also be assured that the problem is understood by the recipient party, be it the developer, sponsor or user.
2. Setting of objectives and overall project plan. The objectives indicate the questions to be answered by means of simulation. This is also where the decision should be made weather simulation is the appropriate tool after all. Banks devises a set of rules to support the decision [18, p. 5]: He discourages simulation if ...

- ... other approaches (common sense, analytical methods, experiments) to achieve the desired answers are available.
- ... the required financial or temporal means are not available or the costs for the simulation exceed the benefits.
- ... unreasonable expectations concerning the abilities of simulation exist.
- ... the necessary data base is not available, the system behavior can't be modeled or the simulation cannot be verified and validated.

Assuming the decision to be positive the overall project plan should specify resources, timeline and outputs of the project phases.

3. Model conceptualization. The development of a conceptual model deals with the abstraction of the essential features of the problem into a model. Since the quality of this conceptual model is probably the most crucial part for the success of a simulation study, the topic will be discussed in more detail in Chapter 2.3.1.
4. Data collection. Data collection should be carried out parallel with model development and should be in constant interaction, since the data availability significantly influences the model architecture and vice versa (see also Chapter 2.3.2).
5. Model translation. In order to be able to execute the model on a computer, the conceptual model must be translated into a computer-compatible format.
6. Verified? The verification process assures that the model was built right i.e. is the translation correct. Banks advocates mainly techniques using common sense to perform this step. However, there has been an extensive amount of research about verification and validation processes which will be discussed in more detail below.
7. Validated? Validation is concerned with the question if the right model was built to represent the actual system. The answers are usually provided by comparing the model to actual system behavior. Again, more details are provided below.
8. Experimental design. In this step the actual experiment to be conducted in the simulation study must be designed, i.e. the alternatives or scenarios for the simulation must be determined.
9. Production runs and analysis. The simulation is run and the results are subsequently analyzed in order to derive measures of performance for the simulated system designs.
10. More runs? Based on the results of the previous step the need for additional runs is determined.
11. Documentation and reporting. Banks suggests that the program and the progress of the simulation study should both be documented. Program documentation is indispensable if a reuse of the models or simulations is intended and progress documentation provides a written history of the project and is a valuable steering tool. Finally the results must be edited and reported to the user and/or sponsor.
12. Implementation. The last step, the implementation of the results in the real system, is actually not part of the simulation study but its consequence. The success, however, significantly depends on the quality of the previous eleven steps and the communication between simulation developer and user.

Since Banks advocated the approach described above, application fields for simulation have become more varied and models have increased in complexity. Therefore, more emphasis is put on more generally applicable process structures and more consistent validation and verification of the respective products during a simulation study. A generalized approach for modeling and model validation and verification often referred to in literature is the simulation cycle according to Robert Sargent [27] as depicted in Figure 5.

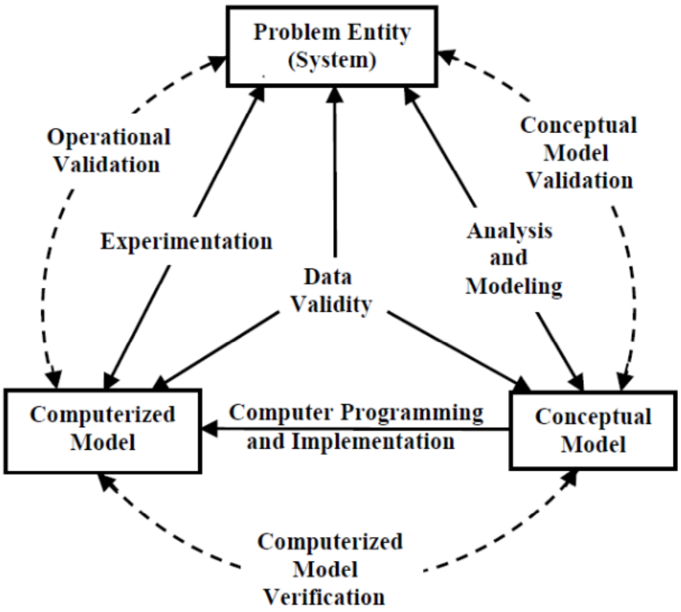

Figure 5: Simplified Version of the modeling process according to Sargent [27]

The problem entity is the system under study from which an analysis and modeling process derives a conceptual model. The conceptual model is the mathematical or logical or verbal representation of the problem entity. Through a programming and implementation phase the conceptual model is transferred into a computerized model. By conducting experimentations with the computerized model conclusions about the problem entity can be drawn. Sargent relates a validation or verification process to each of the three steps in the modeling cycle:

Conceptual model validation determines whether the underlying theories and assumptions of the conceptual model are correct and the model is a reasonable representation of the real system for the intended purpose. As feasible validation techniques Sargent suggests face validation and traces. Face validation makes use of expert knowledge to determine if the model behavior is reasonable. Using traces different types or entities are followed (traced) through the model in order to determine the logical correctness and the accuracy. In a previous publication Sargent especially encourages the use of graphical models for these validation techniques [31]. He also emphasizes that each submodel and the overall model must be examined to ensure appropriate detail, structure and relationships.

Computerized model verification ensures that the conceptual model has been implemented correctly. As a general rule Sargent states that the more specialized the simulation or programming language the fewer errors are likely to happen. If a simulation language is used he suggests on one hand testing the language and its implementation and on the other hand testing if the model was programmed correctly. The preferred techniques are again traces and structured walkthroughs, which are a software peer review technique. If a programming language is used he suggests adopting techniques found in software engineering.

Operational validation ensures that the model output is of sufficient accuracy for the models intended use. A large number of validation techniques are available for this final step of validation. The major aspect for choice of validation technique is if the problem entity is observable i.e. if it is possible to collect data on its behavior. Lack of the opportunity to compare model outputs with experimental data affects the confidence in the model. Therefore, Sargent suggests examining the model output behavior thoroughly with respect to reasonable behavior or comparing the model to other valid models.

Since model errors cannot only be caused by incorrect models but also by the use of incorrect data, Sargent introduces data validation as the fourth validation process. However, he admits that ensuring that data is correct is difficult. Therefore, he suggests ensuring the quality of the processes in connection with data collection, maintenance and testing. Averill Law also suggests that the modeler needs to communicate clear specifications of the data requirements and vice versa needs to understand the processes that produced the data [25].

Complementary to Sargent's process description a variety of literature concerning appropriate choice of validation and verification techniques for every process step is available, such as [32], [33]. Furthermore, useful techniques for objective validation with limited data resources are presented in [34], [35].

Apart from validation and verification techniques Sargent has also taken into consideration the role allocation. Commonly the simulation team itself decides if a model is valid or not. Sargent suggests that preferably this decision should be left to the simulation result users or an independent party, especially if the simulation team is small.

Besides from being valid and verified Law also sees an important aspect of a model in its credibility [25]. He defines credibility of a model and its results if the decision makers and other stakeholders accept the model or its results as correct. Credibility does not imply validity or vice versa. It is dependent on other factors apart from validity, such as: decision maker's attitude towards the model (insight, involvement in the process), reputation of developers, presentation.

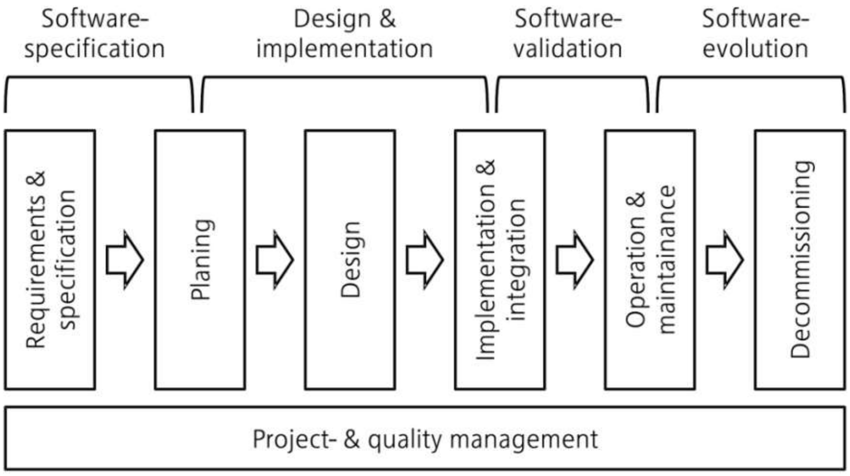

Figure 6: Software Life Cycle according to [36, p. 13]

With even more growing complexity in recent years large simulation studies require a process structure more comparable to life cycle approaches used in software engineering (see Figure 6). Osman Balci has formulated a life cycle for modeling and simulation which identifies processes and work products and a complementary credibility assessment [28], [29]. The life cycle consists of 12 processes of which are depicted in Figure 7.

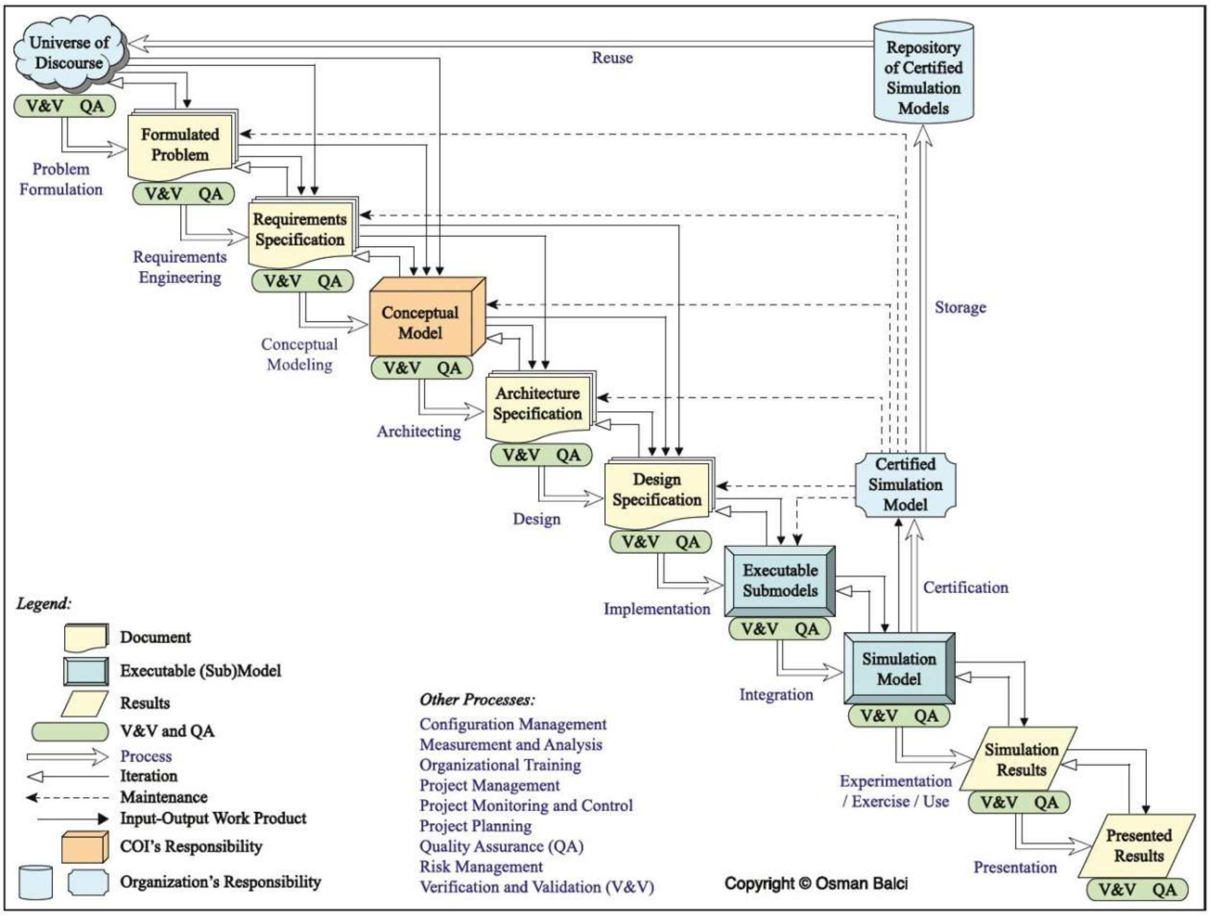

Figure 7: Life cycle for modeling and simulation according to [28]

According to Balci the life cycle provides a framework for guidance for model and simulation development teams. It is also meant to be of iterative nature with processes undergoing repetitions until the desired qualities of the work products are achieved. Every product of the simulation cycle is subject to validation, verification and quality assurance. Balci also puts great emphasis on the first steps from problem formulation until implementation for which he has developed detailed step by step guidelines and checklists.

The problem formulation according to Balci is a step often not given enough attention by modelers. It greatly affects the credibility of the results because it assures that the actual problem is identified. Furthermore the problem formulation or definition specifies the problem boundaries, relevant stakeholders, constraints, objectives and data as well as information structures.

The requirements specification identifies the requirements to the simulation by assessing the stakeholders modeling and simulation needs and their feasibility, specifying the intended uses and use cases and finally deriving the requirement specification. Intended uses refer to the purpose for which the simulation is intended and can fall under categories like analysis, comparison, evaluation, control, optimization, etc. Use cases specify the behavior of a model and are descriptions of sequences of actions a model performs to produce observable results. A more detailed description of the stages of the requirements engineering process was previously published by Balci in [37].

The next stage is the conceptual modeling. Balci characterizes a conceptual model as *repository of high-level conceptual constructs and knowledge in a variety of communicative forms (e.g. animation, audio, chart, diagram, drawing, equation, graph, image, text, and video) intended to assist in the design of any type of large-scale complex M&S application*.[28], [29]. A detailed discussion on Balci's approach to conceptual modeling can be found in [38].

The next step to further substantiate the model is the process of architecting which specifies the organization of the modeling and simulation applications based on the conceptual model and the requirement specification. As a standard architecture Balci suggests High Level Architecture [39], Client-Server Architecture or Distributed Objects Architecture.

After the architecture the design of the model is specified. The design process uses decomposition and modularization in order to handle model complexity and delivers a quite detailed design specification which determines for instance the modeling approaches (continuous, object oriented, Monte Carlo,…).

Using the design specification as an input the executable sub-models are implemented and integrated into the simulation model. Balci sees the modeling stages conceptual model – architecture – design – executable models as layers of model abstraction, with the conceptual model as the most abstract to the executable simulation model as the least abstract. After the successful implementation, follow the life cycle phases of experimentation with the model, presentation of results, (optional) certification, storage, and (optional) reuse.

Facing this rather complex process it might be worth noting that Balci's research derives from military background where very large modeling and simulation processes are managed and integrated.

2.3. Models

After describing the modeling and simulation process in general this section will go into some detail about the conceptual models underlying simulation studies in order to provide a basis for the remarks in the following chapters. As discussed above there are fundamentally two types of models: conceptual and computerized models. Computerized models are executable in some form on a computer. They will not be discussed here in further detail because their properties are mainly dependant on the executing simulation environment or computer program. Conceptual models are the theoretical basis for computerized models and will be discussed here in detail. Further on as a somewhat transitional step from conceptual to computerized models the basic mathematical modeling approaches will be summarized.

2.3.1. Conceptual Models

Conceptual models are one of the core concepts of simulation studies and still there is surprisingly little literature on the general approaches to modeling. Maybe this is due to the fact that modeling is considered more an art than a science [26]. This point of view might explain a lack of literature dealing with the formalization of modeling processes. It seems like the 'art' of modeling is still mostly acquired by experience [40]. However, a hand full of papers has dealt with the challenge to provide at least a rough guideline to this art over the last decades.

First dispute is over the definition of a conceptual model. As discussed above Balci describes the conceptual model as *high-level conceptual constructs and knowledge in a variety of communicative forms* [28]. This, however, seems to interfere with Sargent's approach according to which the conceptual model directly translates into the computerized model [27]. The most quoted definition of conceptual models origin from Robinson, who defines a conceptual model as...

> *... a non-software specific description of the computer simulation model (that will be, is or has been developed), describing the objectives, inputs, outputs, content, assumptions and simplifications of the model.* [41]

According to this definition, a conceptual model is some sort of abstraction of the system under study. It is widely agreed in literature that getting the amount of abstraction right is the real art behind conceptual modeling. Still Robinson's definition does not include every necessary specification between system under study or real system and the computerized model, as does Sargent's definition. Therefore he introduces system description and model design, which he still defines as parts of the conceptual modeling process. The relationship between these concepts is shown in Figure 8.

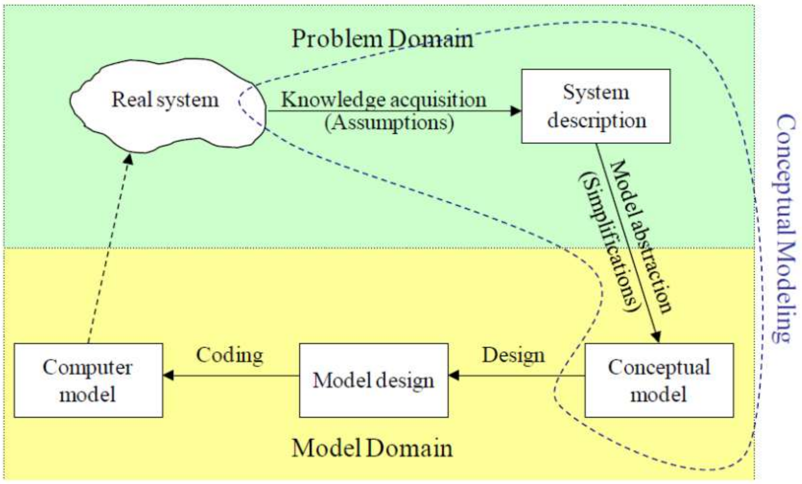

Figure 8: Artefacts of conceptual modeling according to Robinson [42]

According to Robinson's survey [43] most literature on conceptual modeling origins from military modeling and simulation applications. The majority of the research was conducted or supported by the US Department of Defense (Balci, Pace) but also some European institutions have undertaken efforts in this direction [44]. However, most modeling and simulation applications in this domain are very large scale and therefore in many cases the concepts for conceptual modeling proposed for these application are overly sophisticated for use in small to medium scale efforts usually found in research projects. Apart from the military domain the literature on conceptual model development is quite limited.

In order to break the art of modeling down to more reproducible scientific processes some researchers, including Robinson himself, tried to formulate general frameworks for guidance. Robinson's framework [42] firstly defines the key requirements of a 'good' conceptual model. It should be valid concerning the results, credible for the clients, feasible to build with the given resources and it should be useful. This leads him to the conclusion that the best solution is to build the simplest model possible to meet the objectives of the simulation study, because simple models

- can be developed faster,
- are more flexible,
- require less data,

- run faster,
- can be better understood and therefore easier interpreted.

Robinson also supports this approach by the statement that with increasing levels of complexity models decrease in accuracy. Trčka explains this phenomenon with complex models requiring more input data and, therefore, the errors caused by flawed data outweigh the benefits of more accurate models [45]. Based on this very realistic approach Robison suggests a conceptual modeling framework which involves five roughly consecutive activities:

- Understanding of the problem situation
- Determining the general project and modeling objectives
- Identifying the model outputs
- Identifying the model inputs
- Determining the models content, identifying assumptions and simplifications.

After performing these steps all specifications required by the definition of the conceptual model are determined. For documentation Robinson proposes templates [42] and a combination of component lists, process flow diagrams, logic flow diagrams and activity cycle diagrams [46, p. 71]. Apart from those, he summarizes a range of methods proposed in literature, which range from petri nets, event graphs, Unified Modeling Language (UML) and object models to using the visual display applications of simulation software environments [43]. However, Kop and Mayr point out that the singular use of graphical languages only show parts of the information needed to develop a system [47]. Therefore, a combination of approaches seems appropriate.

Complementary to Robinson's approach a few other frameworks for model development have been published. Nance introduced the conical methodology [48], an object oriented approach that proposes a combination of bottom-up and top-down approaches for model specification and definition. The methodology furthermore stresses model decomposition, characterization of the simulation objects (submodels) by attributes and introduces a taxonomy for the attributes which relates all attributes back to eight fundamental types which are shown in Figure 9.

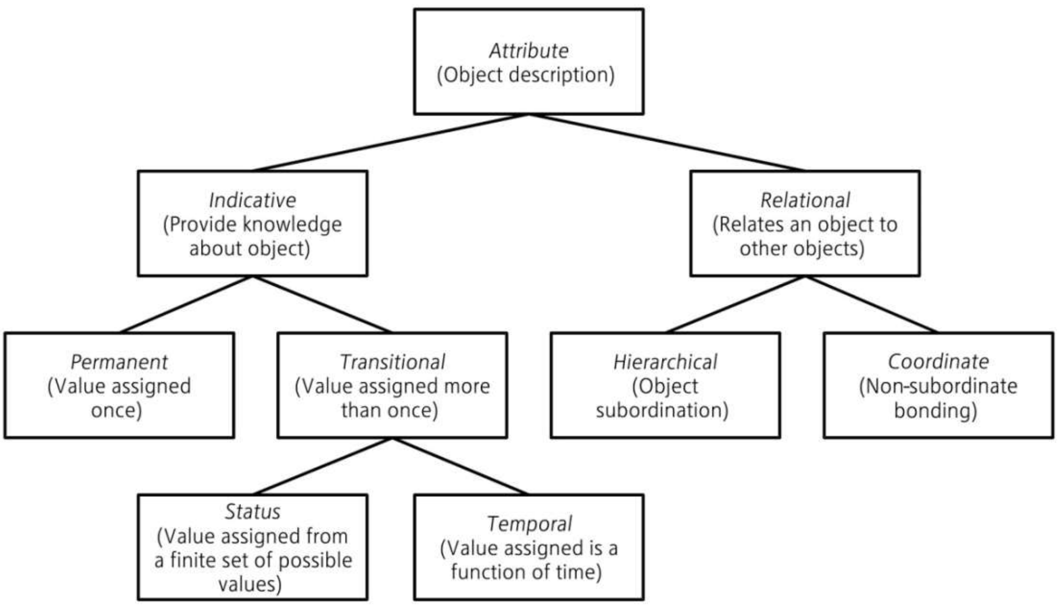

Figure 9: Attribute types according to R. Nance [48]

Pace published a four step approach to conceptual modeling [49]. It leads from collecting of authoritative simulation and context knowledge over identifying entities and processes to developing of simulation elements and finally to addressing relationships between the elements. Furthermore he provides a guideline for model decomposition in order to determine the simulation elements to be included in the model:

- Every item specified for representation by the simulation requirements should be represented by an item. This ensures the requirements can be translated to specifications.
- Every item of potential assessment interest should be represented by a simulation element. This ensures the potential use of the simulation and its measures are understood.
- As far as possible every simulation element should have a real world counterpart.
- Whenever possible, the simulation elements should correspond to accepted decomposition paradigms to ensure acceptance and effective interaction.
- Simulation elements that do not meet the previous items but are required for computational considerations should be used only when absolutely necessary.
- Extraneous simulation elements should be left out.

Other researchers focused on the development of methodologies and frameworks for conceptual modeling for specific application fields. Van der Zee embeds conceptual modeling into an engineering process and aims specifically at providing a solution that facilitates interdisciplinary collaboration, which is often encountered in engineering projects [50]. Guru and Savory have formulated a template based modeling infrastructure for a case study of physical security systems, that could also find application in other areas of discrete event simulation [51]. Birta and Arbez [23] as well as Furian [52] developed conceptual modeling frameworks for discrete event simulation. However, no literature for conceptual models specifically targeted at continuous systems could be found.

Some research focuses on conceptual modeling as a tool for knowledge acquisition and communication between the stakeholders of a simulation study. According to Shannon [26], there are two kinds of knowledge or skills needed in a simulation team. First knowledge and understanding of the system under study is required and second modeling and simulation skills as well as knowledge about statistical analysis and data collection are required. The first is usually contributed by subject matter experts (SMEs) or domain experts the latter by M&S designers. Balci [53] sees conceptual models as an important communication tool among these two groups of people which therefore also play an important role in reuse of modeling and simulation applications. Setavoraphan and Grant consider conceptual simulation modeling as a possibility to structure domain specific simulation environments [54]. Research around Kathy Kotiadis focused on the process of knowledge acquisition from SMEs for the system description and model abstraction [55]–[57].

2.3.2. Mathematical Models

From the pure conceptual model mathematical models bridge the gap to computerized models and form a part of the model design. Mathematical models can be categorized by different characteristics resulting from the system behavior and the accordingly chosen modeling approach. Understanding of these fundamental principles of modeling is vital for model development but also proves to be helpful for the design process of the conceptual models and for the communication of domain experts.

The first major characteristic of models is whether they incorporate time dependent behavior or do not i.e. are "static". Time dependent behavior in this context is in many domains referred to as "dynamic". However, in plant and energy system simulation a more detailed subdivision, to the term is applied, as summarized by Wischhusen in [58, p. 5] for continuous time models (see below):

Static or steady state models are described by an algebraic system of equations f_{ae} with the internal variables x_a that characterizes the model is only dependent on the inputs $i(t)$, which are constant during the simulation time Δt, in order to calculate the outputs o.

$$f_{ae}(x_a, i, o, t) = 0 \qquad \text{with} \qquad i(t) = \text{const} \quad \text{for } \Delta\text{t} \tag{1}$$

What is often referred to as dynamic models is called "unsteady" or "transient" and divided in two subcategories: "quasi stationary" models and "dynamic" models. Quasi stationary models describe processes in systems that can be approximated by a series of thermodynamic equilibriums. The model consists of an algebraic system of equations f_{ae} like the steady state model, but in case of a quasi stationary model, the inputs $i(t)$ are not constant during the simulation time. The unsteady behavior of the system is exclusively induced from the environment. Changes in the model state due to storage effects are not considered.

$$f_{ae}(x_a, i, o, t) = 0 \tag{2}$$

Dynamic models: These models are described by a differential-algebraic set of equations f_{dae}. The quasi stationary processes represented by the algebraic equations are set into balance with the dynamic model part with the dynamic states x_d. Dynamic models do incorporate storage effects.

$$f_{dae}(\dot{x}_d, x_d, x_a, i, o, t) = 0 \tag{3}$$

In this thesis from this point on "dynamic" will be used to characterize models structured according to equation (3) and "transient" for models according to (2) and (3).

The second aspect that distinguishes transient models is the behavior of their state variables over time. These can either show continuous- or discrete-time behavior. Cellier characterizes continuous-time models by the fact, *that within a finite time span, the state variables change their values infinitely often* [17, p. 11]. Figure 10 shows the trajectory of a state variable of a continuous-time model.

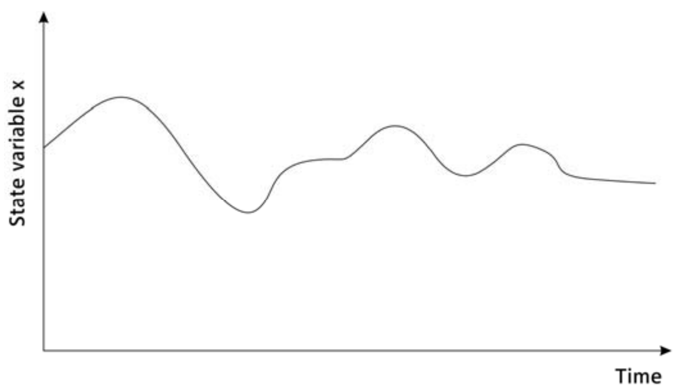

Figure 10: Trajectory of a state variable of a continuous-time model

As described above dynamic continuous time models are usually described by differential equations. Among these models two further classes can be distinguished: lumped parameter models and distributed parameter models. Lumped parameter models concentrate the physically distributed quantity in one variable or point i.e. the space variables are discretized. They are described by ordinary differential equations. Distributed parameter models describe a physical distribution of a quantity and are described by partial differential equations.

In discrete-time models the state variables change their value only at certain points of time. They are frequently used to describe computer controlled systems. Due to the fact that computer algorithms take time to calculate control signals a continuous operation is impossible and therefore intersecting the time axis i.e. discretizing it is a logic implication. Discrete models are often represented by difference equations. Figure 11 shows the trajectory of a state variable of a discrete model.

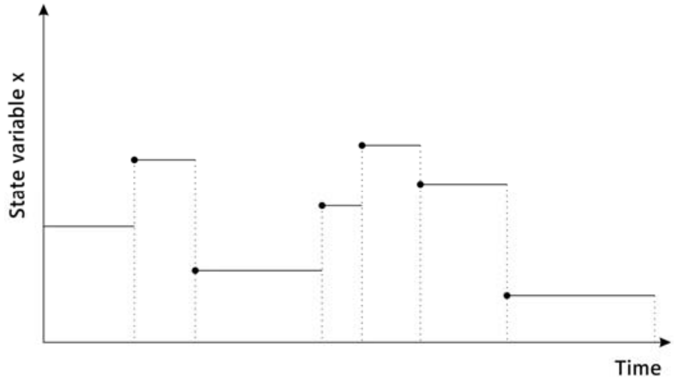

Figure 11: Trajectory of a state variable of a discrete model

Note that because of the characteristics of computers, every continuous model must undergo a certain discretization in order to be simulated on a computer. All the previously mentioned models assign variables a numerical value and therefore are called quantitative models. A subclass of discrete models are qualitative models. The dependent variable is also discretized into a finite set of values or classifications (e.g. grading of students).

An import aspect of the nature of systems and their corresponding models is determined by their in- and outputs. As mentioned above systems possess inputs and outputs. Inputs are variables that influence the system from the environment. Outputs are variables that are determined by the system behavior. This is equally true for the models of systems.

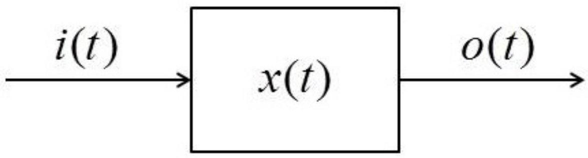

Figure 12: Block diagram of a system

If for a model all inputs $i(t)$ are known and the outputs $o(t)$ can be calculated, using the internal variables $x(t)$ the model is called causal. But for many models the same variables can act as inputs or outputs. This model behavior is called acausal. It is the case for physical systems if exchange of a quantity influences the state of the system, but the state of the system influences the same quantity exchange e.g. voltage – current, temperature – heat flow.

Another distinguishing feature of models is the type of information used for the construction of the model. As presented by Karplus in [59] the available information about the system has a determining impact on the model design, structure, validation and credibility. There are two types of information a model can be based on: knowledge about the system that is being modeled or data about input – output relationships of the model. A modeling process based on the former type of information is executed deductively while the latter form of information requires an inductive process.

In a deductive modeling process the mathematical model is derived analytically, using knowledge of the system's structure, the underlying (physical) laws and parameters. The construction of a valid mathematical model purely by deduction requires the knowledge of all components of the system and their connections. According to this transparency of the underlying system the model is dubbed white, clear or glass box model. Due to the nature of deduction a model constructed this way presents a unique solution of the modeling problem.

Contrasting to the deductive approach, an infinite number of inductive models can satisfy a given data set. In an inductive modeling process the inputs and outputs of the system are known and the mathematical models must be derived from them. Because of the obscured view on the system this type of representation is called black box model. Therefore, quantity and quality of the available data are determining for the validity of the model. This is especially critical, if the modeler cannot actively chose the input and conduct an experiment on the system but has to rely on passive observations of outputs at given inputs. The dependency on observed data rather than system knowledge, however, affects the credibility of the model.

In order to eliminate uncertainty from an inductive modeling process and receive a more credible representation of the system, the input and output data can be supported by whatever information about the system is available. In most modeling tasks the underlying system is not completely unknown, anyway. Therefore, Karplus extends the black and white modeling world to a rainbow of various shades of grey and tries to make some connection to model applications, domains and numerical approaches (see Figure 13). Although some of his categorizations may have blurred or shifted a little since the publication of his work in 1977 with the continuing progress in modeling domains, the general principles are quite useful for the further reflections in this thesis and, therefore, are discussed in more detail.

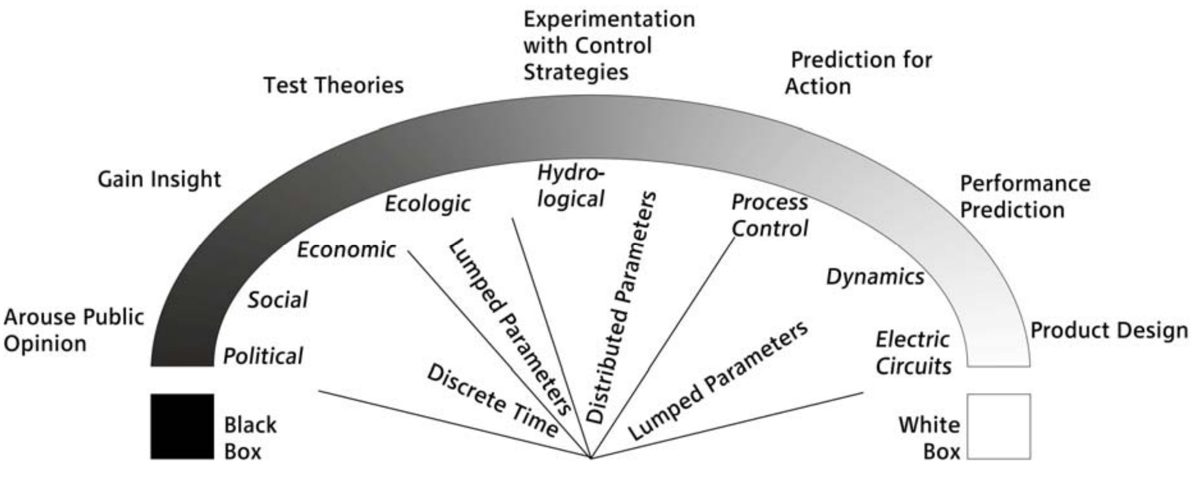

Figure 13: Black box white box spectrum according to Karplus [59]

Concerning domains as a prime example for white box modeling Karplus puts electrical circuit models on one end of the spectrum. In this discipline usually the structure and all elements of the circuit are known and the models can be inferred using well known physical laws. Moving away from the white end of the spectrum dynamics and chemical process control can be found, where most mechanical principles or reaction equations are known, but parameters may have to be supplied from experimental data. Further in the grey spectrum he puts hydrological phenomena as an exemplary field for diffusion processes, which are well described by partial differential equations but the properties of the media are often imprecisely known. Physical laws underlying life science models are even less explored and on the dark end of the spectrum even basic principles governing the dynamic behavior and system interdependencies are subject of debate in economic, social and political systems.

Karplus furthermore postulates that the respective shade of grey a model finds itself in implies a *built-in "validity factor"*, which in turn means that the purpose a model can serve must conform to its expected validity and ultimately the chosen modeling approach. White box models are an important tool for product design or can be used for precise prediction of system behavior. Closer to the black box side he sees models that provide a general insight into the system in order to explain often counter intuitive behavior. The primary objective in some models he sees in simply arousing public opinion and therefore their conclusion must be more on the qualitative side. Based on Karplus, Cellier more blatantly categorizes the application cases from white to black as: design – control – analysis – prediction – speculation [17, p. 15].

Last but not least he assigns different degrees of discretization to different purposes and application fields (see Figure 13). This categorization may be a little dated in some areas with the progress in computer and simulation technology. Distributed parameter models are for instance state of the art for design processes nowadays.

2.4. Building Performance Simulation

In the development cycle of engineering products usually simulation follows concept development, calculation and design for in depth investigation of certain aspects of the product. Afterwards a prototype is constructed for proof of concept before the serial production of the finalized product design is started. In the building sector the prototype is usually the finalized product. Serial production of buildings is generally not the norm. Therefore the important step of proof of concept is passed by. This creates the need of even more careful theoretical analysis of the planned product and assigns an even more important role to simulation.

Building performance simulation is an area that includes a variety of aspects studied and researched in the context of buildings. One aspect that is, however, generally agreed on, is the fact that it deals with resource - mainly energy – flows in the building. One of the main cores of building performance simulation is the building simulation itself which is usually focused on energy flows i.e. a thermal simulation. Other aspects include the occupant behavior, lighting, hygienic conditions, special aspects of comfort, control, etc. Another main aspect of building performance simulation, which is in literature often summarized under this term, concerns itself with the energy system attached to the building. Models of the building energy systems usually include all on-site devices that convert, distribute and supply energy for the building and its users. This includes usually thermal energy for heating and cooling purposes, electricity for operation of devices but also process heat and cold and otherwise converted energy (e.g. pressurized air). Systems can range from very small and straight forward systems relying only on one or two energy supplies to cover all user demands as often found in households to highly complex systems featuring a variety of conversion units, storages and distribution networks as employed by large public facilities or industrial plants. Sometimes renewable energy sources are integrated too. Simulation of such systems, focusing on the system behavior aspect, not on individual components, appear in literature under different names e.g. building energy system, HVAC systems, hybrid energy systems, distributed energy systems, etc. In this chapter the term building performance simulation (BPS) will be used to summarize all the above mentioned aspects if not specifically indicated otherwise.

Building performance simulation has its root in the 60th of the last century [60] and has since then evolved into a prospering field of research. Tools have undergone a development from very simplified analytical methods to numerically operating instruments often fully integrating several of the above mentioned aspects of BPS.

Traditionally the main application field of building performance simulation was during the design phase in the building life cycle. It has proven to be a valuable tool to compare design options and many researchers have stressed the benefits of applying simulation in the design phases [61]–[63].

In recent years the application fields of building performance simulation moved beyond the design phase and extended to commissioning and operation. Building performance and energy system simulation can be a valuable tool to address gaps between predicted and actual performance of a building, assist in the development of business models based on the whole life cycle performance of buildings and determine operation strategies for existing structures. Out of this shift in application new research questions arise. Clarke and Hensen [64] identified twelve research areas that are recently being pursued with increased effort:

- **Air Flow** Building Performance Modeling is often applied to develop ventilation strategies and ensure air quality and comfort indoors. Therefore the integration of models for detailed air flows prediction started decades ago. Network air flow modeling has been implemented in the 1980. More recently the application computational fluid dynamics has been subject of investigation [65], [66].
- **Lighting** In the context of daylight simulation Clarke and Hensen see the challenge addressed in research in the past years in modeling the rapidly changing sky brightness distribution with a feasible numerical effort.
- **HVAC Systems** A lot of work was contributed to building libraries of dynamic models for HVAC simulation e.g. [58], [67], [68]. Especially with object-oriented, equation-based modeling approaches the synthesis of component models from basic elements and the rapid configuration of particular instances are facilitated.
- **Control** Simulation assisted control has been a rapidly growing field of application for building simulation in recent years [69]. Afram and Janabi-Sharafi published an extensive review of model predictive control for HVAC systems and conclude that model predictive control offers superior performance in comparison to conventional controllers [70]. A number of case studies concerning MPC applications can be found in literature [71]–[74].
- **Occupant representation** Occupant behavior has been recognized as one of the determining factors for the energy performance of buildings. Therefore, a number of studies have assessed the impact of user behavior on the energy performance of the building [75]–[77].
- **Model quality assurance** Concerning correctness of models and therefore credibility of simulation results has been some debate. But several researchers showed that, given careful editing of input data, simulation results are of satisfying accuracy [78], [79]. As a unified effort to introduce quality assurance ASHRAE released the standard 140 which specifies a method of test for evaluation of building energy analysis [80].

- **Uncertainty considerations** A major challenge in building simulation is how to deal with uncertainties in simulation inputs (especially user behavior) and the resulting outputs. There are two ways to deal with this: either sensitivity analysis or embedding an uncertainty model in the program algorithm. [81] provides an overview of the current state of the art in this field.
- **Exergy analysis** Most conventional building performance simulation provides analysis based energy balances. But recently some simulations of builds and HVAC systems also made attempts to carry out exergy analysis for the systems under study [82]–[84].
- **Computation time** Computation time of building performance simulations is an issue for feasibility of real-time applications. Clarke and Hensen see efforts being made to address this problem by solver development and model reduction. By now frameworks for real-time building performance monitoring and comparison to simulation results have been developed and successfully tested [85], [86].
- **New and renewable energy systems** Modeling of renewable energy systems with high fluctuation requires on one side the development of demand side management systems [87] and algorithms and on the other side models for renewable energy technologies [58], [67].
- **Intelligent front- and back-end** The integration of simulation tools into the design process has been an issue of discussion and investigation for some time [88]–[91]. Furthermore Clarke and Hensen point out that the requirements for output data vary widely with the expertise of the tool users and therefore further encourage the development of intelligent front- and back ends.
- **Economic considerations** Accurate estimation of the cost of the implementation of low carbon technologies are difficult and therefore are excluded of most building performance simulation software packages. However, life cycle cost estimations based on simulations have gained increasing popularity in recent years e.g. [92], [93].

Facing increasingly more complex systems a further step in building performance and energy system simulation as identified by [94] would be the combination of different tools in a way that the integrated results provide added value to the user. This can be achieved by linking applications at run-time, the so called cooperative simulation or co-simulation, which will be described in more detail in 2.5.

Since the main focus of this thesis lies on energy systems modeling an excellent overview of approaches and tools in this sector published by Marija Trčka [45] shall be summarized and complemented here. Trčka categorizes the available tools with respect to the problems or aspects of the system they are meant to deal with or otherwise speaking the intended uses of the results.

- **Tools for pipe/duct and equipment sizing** are system design tools that do not necessarily reflect transient behavior. Equipment sizing tools are usually based on calculation algorithms by ASHRAE or are proprietary tools by equipment manufacturers.
- **Tools for energy performance analysis** predict the annual energy consumption of the system. Based on system equations they analyze full- and part load performances at fixed time intervals (e.g. hourly). Best known examples are DOE-2 [95], EnergyPlus [96], ESP-r [97], IDA ICE [98], TRNSYS [99]. Models provided in these tools are of dynamic nature.
- **Tools for system optimization** are in conjunction with tools for energy performance analysis used to modify a set of parameters according to an objective function. GenOpt [100] is an example.

- **Multi-domain simulation tools** can be used to build and simulate models of building energy systems as well. Although not specifically targeted for building energy systems and therefore not included in Trčka's list, this option has gained popularity over the last years. MATLAB/Simulink and Modelica/Dymola offer component libraries targeted at this application field and especially Modelica has gained high popularity [101]–[104].
- **Tools for control analysis and optimization** are highly dependent on the level of abstraction of the controller model. While performance analysis tools all include models for control strategies of some degree of abstraction or simplification, for detailed representation of controllers usually multi-domain tools like MATLAB or Dymola are used.
- **Simulation tools for real-time performance optimization** can be used for a variety of cases such as diagnostics, emulation of the building or HVAC systems to test system responses and simulation assisted control. Generally all tools for performance analysis and multi-domain simulation can be used for this. But literature gives the impression that Modelica and TRNSYS are generally preferred.

Sinha and Chandel [105] and Crawley et al. [106] have published extensive reviews of software tools for building performance simulation comparing the specific aspects and characteristics. However, it needs to be considered that the requirements on software tools vary with the intended use and the domain of the user, as demonstrated by Attia et al. in a survey among engineers and architects [107].

Concerning co-simulation a framework specifically targeted to the needs of building performance simulation was developed at the Lawrence Berkley National Laboratory [108]. The Building Controls Virtual Test Bed (BCVTB) integrates MATLAB, Dymola, EnergyPlus, Radiance, ESP-r, TRNSYS and BACnet, the data communication protocol for building automation by ASHRAE, for hardware in the loop applications.

2.5. Simulation of Complex Systems, Cooperative Simulation

In recent years systems increasingly gained in complexity and interactions with other systems became determining aspects for system design and operation. In literature these large systems, comprised of a number of interacting, heterogeneous components are often described as "complex systems", "hybrid systems". Siegfried describes as a key property of complex systems that no single component controls the system behavior [109]. Some are even characterized as "system of systems (SoS)", if the subparts can be used independently and integrate along the value chain [110, Ch. 1.3] or are associated with different disciplines and experts [111, p. 7]. Traditional simulation methods reach their limitations to answer global questions about these complex systems. With different disciplines and views involved the submodels are often heterogeneous and must be integrated into a composite model. According to Popper a number of different terms are used for this kind of modeling, such as "hybrid modeling", "coupled modeling", "interconnected simulation", "interfaced simulation", "integrated simulation", "multi-method modeling" and many others [22, p. 70].

In the area of building performance and energy system simulation integration of different systems has gained significant popularity as well. This includes classic co-simulation as well as the integration of virtual and physical components in one system under study and is mainly due to current trends in the research field (see also chapter 2.4). Ambitious energy efficiency benchmarks require a more thorough investigation of relevant aspects in the building. This demands the integration of tools to assess specific aspects of the building performance, such as indoor air movements or lighting. Examples can be found in [65], [66], [112]. The goals to include renewable energy sources in the grid requires new assessment tools to investigate the grid behavior, to couple it with models of fluctuating energy sources and also to integrate and eventually manage the user behavior [113], [114]. Another currently emerging field of research are simulation assisted operation strategies buildings and energy systems which require integration of real and virtual systems [69], [86], [102].

If only modeling and simulation tasks without hardware are concerned, different solutions to model different domain subsystems in different tools exist. Cooperative simulation or co-simulation in some definitions is strictly the coupling of two or more models implemented in two or more different modeling tools and executed in two or more distinct solvers [115, p. 18]. Other sources apply more open definitions that also call the coupling of solvers in one simulator co-simulation. The use of two different simulators is specified as external coupling [116, p. 21]. In any case distributed simulation refers to the integration of simulators running on different physical machines. According to Völker [115, p. 57] co-simulation in its present form was developed in the early 1990th and offers three main advantages compared to monolithic solutions:

- Modeling advantage: Different Disciplines can be modeled in modeling tools optimized for the specific purpose
- Engineering advantage: Speeding-up of the engineering process by parallel modeling of the different subsystems
- Efficiency advantage: Each Solver can integrate his subsystem with ideal time discretization

When coupling simulations in a co-simulation a number of forms of numerical exchange of variables between the models can be realized. The different types are described into more detail by Hafner [117, p. 24] and Trčka [116, p. 33].

Firstly two different kinds of simulator execution must be distinguished. Methods with discontinuous simulator runs feature one simulator that pauses at certain time steps and calls an external simulator, which performs a run based on data supplied by the first simulator and feeds data back to the first simulator, which again proceeds with the simulation until the next pause where the process is repeated. The second method is the continuous simulator run, where the coupled simulators are synchronized and exchange data at certain time-steps.

Secondly different kinds of coupling strategies can be defined. Strong coupling requires an iteration procedure at every exchange step until user defined convergence criteria are satisfied. Loose coupling only requires the simulators to exchange data at certain time-steps, whereby the needed values have to be extrapolated from the previous values.

For loose coupling two different methods of data exchange can be applied. With the Jacobi-Type the simulation of both systems takes place simultaneously and variables are exchanged at the end of every time step. Hence the variables of both systems must be extrapolated for the next time step. With the Gauß-Seidl-Type the simulation of both systems takes place consecutively, which means that for the successive system the exchanged variables can be interpolated. Figure 14 shows a graphical overview of the coupling methods, whereby circles depict subsystem's states at certain time steps, full line arrows indicate simulation progress and dashed arrows variable exchange. The Gauß-Seidl-Type is more accurate, especially with stiff systems, but slower than the Jacobi-Type. In order to treat stiff systems, it is also possible to vary the length of time steps of the different simulation models. This so called multi-rate simulation can be utilized to vary the coupling sequences of the Gauß-Seidl-Type as demonstrated in more depth by [116, p. 37]. Furthermore some thought should be put into choosing the system integrated first. With the "fastest-first" method the stiffer system is integrated first which results in more accurate results but the need for smaller time steps i.e. more storage demand. The opposite is true for the approach of integrating the slower system first.

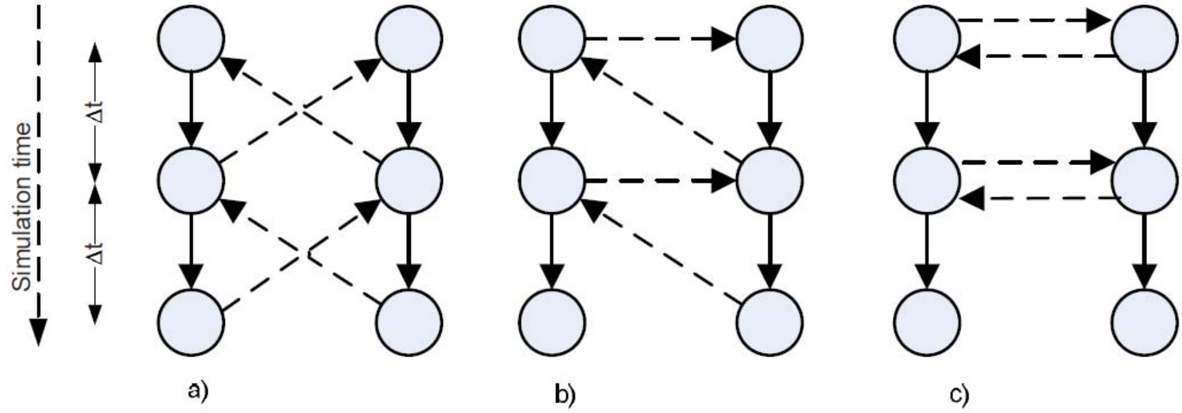

Figure 14: Data exchange methods: a) Strong coupling b) Gauß-Seidl-Type c) Jacobi-Type. Circles depict subsystem states at certain time steps, full line arrows indicate simulation progress and dashed arrows variable exchange [116, p. 35]

During a co-simulation every simulator solves his own model, but in order to ensure the coordination, i.e. the exchange of simulation variables during the run-time a superior controller and data exchange interfaces are needed. The data sharing processes between the simulators can be organized by interprocess communication protocols. An overview of the most commonly used ones for building performance simulation purposes is given by Yahiaoui [118]. The role of the simulation controller can either be dedicated to one of the simulators involved in the simulation or to a separate co-simulation engine or framework. Figure 15 depicts the general architecture using a co-simulation engine for the example of a discrete-event (DE) and continuous-time (CT) simulation coupling. During the simulation run the engine is responsible for exchange of simulation variables, event passing and time step coordination.

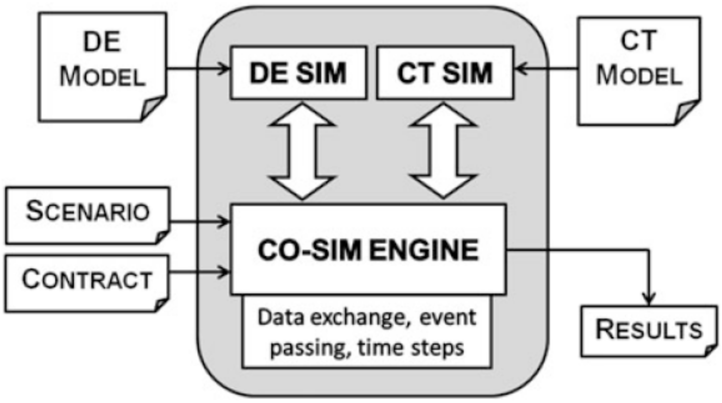

Figure 15: Co-simulation engine for discrete-event and continuous-time simulation coupling [119]

As mentioned above the Building Controls Virtual Test Bed (BCVTB), developed by the Lawrence Berkeley National Laboratory offers a co-simulation engine for building performance simulation applications [108].

One core question of co-simulation that takes all the above mentioned into account, is where to partition the model or in other words where to interface the simulators. According to Vaculín et al. [120] a few aspects should be taken into account, which include:

- Workflow aspect: Uni-directional interfaces are needed if one program acts as a pre-processor for a second program. Bi-directional interfaces exchange data between two running simulations. Therefore at least some results are available for both tools. The latter is usually the case in co-simulation
- Mathematical and physical aspects: For allocation of interfaces the form of the model (data model, physical model, black box model) and the model size i.e. the degree of reduction should be taken into account. Furthermore the numerical integration of the interfaces i.e. which and how the data between the simulators is exchanged (see above), is an important aspect to consider.
- Software, hardware and implementation issues: Another concern to be weighed is the choice of simulator and the according model integration or translation, the technical aspect of data exchange and whether to run the co-simulation on a single-platform or distributed.

2.6. Related Work

In this chapter theses of three colleagues will be presented. These particular theses have been chosen, because the research presented in them was either done in close cooperation with the author or because the results have been used for the work presented in this very thesis.

Path towards Renewable Energy Supply – Holistic Optimization of Supply Chains by Application of Advanced Engineering Methods [121]

Dietrich Wertz describes in his PhD thesis models for building-related energy converters and storage systems and presents simulation results for reference sites and reference periods. Apart from technical issues the focus is put on legal and economical boundary conditions. The aim of the thesis was to identify measures, which have to be adopted at all levels (energy production, distribution and end-use) to reach a "socially ideal" energy system. Only a holistic solution can lead to this point. Wertz formulates recommendations concerning building hulls, storage systems, energy grids and energy converters.

The work also shows that in addition to further advancing technologies which are already available today, holistic approaches become more and more important because the complexity of buildings is increasing: This applies on the one hand to each stage of a building’s life cycle (planning, construction, maintenance) and on the other hand to each discipline involved in the establishment and maintenance (spatial planning, architecture, building physics, facility management).

Findings from several research projects are incorporated into the work. Relevant for this thesis are mainly the outcomes of the project ADRES, in which a library for decentralized energy converters was created. Some of these models were adopted and adapted for the projects that lead to this thesis.

Comperative Modeling and Simulation – A Concept for Modular Modeling and Hybrid Simulation of Complex Systems [22]

Niki Popper developed approaches to handling modeling and simulation tasks of complex systems during years of practical experience in the field of simulation, which he has summarized in his thesis. Based on established methods for modeling and simulation he developed a concept for extending the modeling process, as well as to analyze, evaluate and compare strategies in the implementation of simulation projects. Popper also compares different modeling methods and identifies differences and equivalence. He makes the assumption that different modeling methods for a system under study (and their subsystems) exist, and should be considered taking into account available data, system knowledge and question of research. Further on the author modifies the modeling and simulation process by integrating these concepts. The developed methodologies are demonstrated at hand of simulation projects in varying domains.

Among others the author uses the project BaMa as a reference for his concept, in which he collaborates as well. In some areas the findings of Popper's thesis are comparable and in some areas complementary to the work presented in the thesis at hand and therefore can be considered as continuative literature.

Possibilities of Co-Simulation with the Building Controls Virtual Test Bed in the Area of Object-oriented Modeling of physical systems [117]

Irene Hafner's master thesis was executed within the INFO project. The thesis tests the possibilities of cooperative simulation with the co-simulation tool BCVTB. A building model as well as several machine models were combined. The introductory chapter also gives a good overview of the method of object-oriented modeling of physical systems and different co-simulation methods are discussed. The implementation deals with the synchronization of all simulators in spite of their individual solver algorithms since accurate synchronization is necessary to even enable cooperative simulation. The co-simulation integrates a thermal compartment model for the machine hall implemented in Modelica/Dymola and individual machine models implemented in MATLAB, Simscape and Dymola as well as a Simulink model for temperature control. Besides co-simulating individual machine models with the room model, BCVTB's performance is evaluated and the possibilities and limits of cooperative simulation with BCVTB are summarized.

This master thesis was the first preliminary feasibility study whether the intended co-simulation of a manufacturing company within the INFO project could be executed using BCVTB. Since the outcomes were positive it was decided based on the findings of this work that the simulation could be implemented in BCVTB.

3. Reference Model

3.1. General Considerations Concerning the Reference Model

When I read a technical paper written by an author from whom I have not read anything before, I usually find that I have the biggest problems not with mastering the intellectual challenges that the paper presents, but with understanding the author's terminology and relating it back to concepts with which I am familiar. [17, p. 251]

This challenge described by François Cellier is certainly familiar to most scientists. Especially in multidisciplinary teams understanding each other and forming a uniform idea about the subject under study, the objectives and the path to meet them can be challenging. Therefore, in many cases using some sort of meta-tool in order to facilitate communication can be very beneficial. When referring to such tools in many cases the term "reference model" is used. The Organization for the Advancement of Structured Information Standards (OASIS) defines reference models as follows:

A reference model is an abstract framework for understanding significant relationships among the entities of some environment, and for the development of consistent standards or specifications supporting that environment. A reference model is based on a small number of unifying concepts and may be used as a basis for education and explaining standards to a non-specialist. A reference model is not directly tied to any standards, technologies or other concrete implementation details, but it does seek to provide a common semantics that can be used unambiguously across and between different implementations. [122]

Considering this definition reference models show a certain similarity with conceptual models, which also provide, according to the definitions given in the previous chapter, communicative measures and non-software specific system descriptions and often rely on decomposition techniques. Another definition specifies the reference model as *an information model used for supporting the construction of other models* [123]. Thus, a reference model can contain significantly more than only the description of the system to be modeled, as does the conceptual model. Guiding principles, procedural instructions, role allocations etc. but also a conceptual model can potentially be part of a reference model. In case of an M&S task it seems advantageous to include a conceptual model or specifications about it (e.g. in form of an ontology) in the reference model. However, it must be taken into account that an increasing degree of specification goes hand in hand with loss of reusability. Therefore, a similar approach as proposed by Balci in [53] concerning conceptual models, which substantiates abstract models, step by step, can be applied to reference models to achieve maximum reusability. Taking these considerations into account a reference model for designing models for complex energy systems will be proposed here.

The proposed reference model contains a process description on how to derive a conceptual model and a design model for the simulations from a given problem situation. The proposed approach is in many ways inspired by Balci's modeling and simulation life cycle [28], which is discussed in more detail in Chapter 2.2. However, the original life cycle is modified in numerous ways in order to take specifics into account. Firstly the original life cycle derived from military background and is targeted towards very large modeling and simulation tasks. Therefore, the process is of sufficient complexity, which can be a little excessive for the complexity typically encountered in engineering and science. In order to adjust the process to scientific needs it was significantly simplified and merged with approaches proposed for small to medium scale M&S

tasks. Furthermore, it was taken into account that not only the reuse of models developed according to the reference model should be enabled, but also the reuse of models and simulation knowledge developed and accumulated previously. And thirdly since the scope of the work is specifically targeted towards a certain application area (energy systems) more detailed specifications about the basic concepts behind the conceptual model without restricting the reusability within the scope of the model any further is attempted.

The process described in the remainder of this chapter was developed through execution of research projects in which modeling and simulation of systems with the main scope on energy flows executed in a multidisciplinary team was a core part of the project. The description of the process represents a formalization of the real process executed in the research projects and iteratively improved, considering the lessons learned during the course of the work. Furthermore, at this point it must be remarked that although the described process is sorted according to a certain procedural steps, it is in no way to be seen as linear. In fact, the process is very iterative and it will in many cases be necessary to revisit previous steps and revise them according to later findings.

3.2. Project Initialization, Problem Formulation and Requirement Definition

Literature generally agrees that simulation studies should start with a description of the actual problem to be solved [18], [25], [26], [28], [42], [51]. Most authors also agree that the composition of the simulation team plays an important role for the success of the task. Tako and Kotiadis specifically implement the role definition into the initialization phase of the project [57]. This approach will be picked up for this process description, because experience has shown that clarification of the roles and assessment of the existing knowledge within the project team in the beginning of the project can significantly facilitate the further collaboration and prevent misunderstandings.

According to literature a few key roles can be identified relating to simulation studies [26], [27], [53], [57]. These roles can be clustered into groups concerning an organizational (or expectational) and a competence based point of view. Regarding the organizational point of view, there are two main groups: the simulation team and the stakeholders. The stakeholders are interest groups concerned with the simulation study and its expected results. These groups mainly consist of the users of the results, the simulation sponsors and potentially involved third parties (e.g. consultants). The simulation team consists of people actually working on the simulation study. This includes all tasks regarding the process: modeling, simulating, documenting, validating, verifying and contributing data and information.

The working tasks can be divided among three main groups that are distinguishable mainly by their competences:

- Project managers and/or operational personnel: As in any project, it makes sense in simulation studies to assign organization responsibilities in the project. Processes and competences associated with this task are well defined in operational research literature and shall not be discussed in further detail here.
- Domain- or subject matter experts: This group possesses in depth knowledge about the system under study and concepts and methodologies related to their specific domain.
- Simulation specialists or M&S application designers: This group has expertise in M&S applications, which consists on one hand of the technical knowledge to program and run

a simulation and on the other hand of the skill to formulate adequate models. Furthermore, skills in data collection and -analysis may be required in this group. In other words simulation specialists are domain experts for the domain of modeling and simulation.

Balci et al. draw a very structured picture of the roles of SMEs and M&S application designers concerning a simulation study [53]. Subject matter experts concerning a problem domain from a community of interest (COI) should be employed to specify the content of the conceptual model (CM). On the other side of the conceptual model the application designers are responsible to derive the M&S applications (see Figure 16). Thus, the conceptual model adopts an important role as a communication tool within the simulation team.

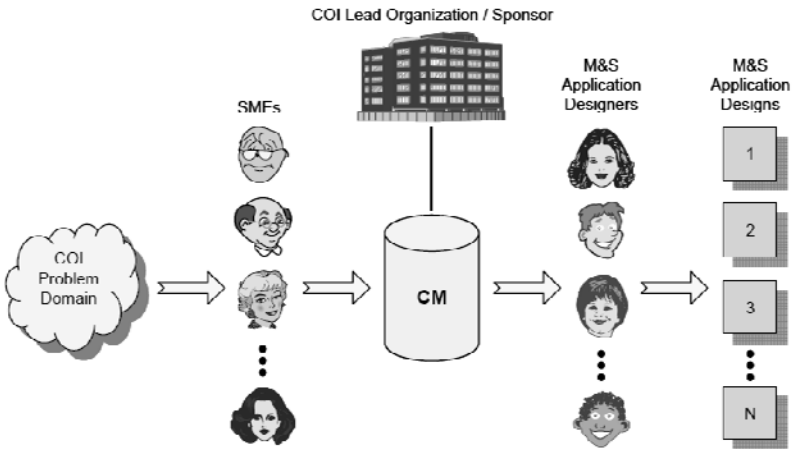

Figure 16: Role of subject matter experts, conceptual model and M&S application designers by Balci et al. [53]

In real life in many cases the distinction between the groups cannot be made with complete accuracy, because frequently individuals unite more than one role in one person. In scientific teams it is often the case that domain experts possess extensive knowledge not only about their respective scientific field of expertise but also about domain specific modeling and simulation techniques. In collaboration with organizations that are the object of study at the same time, the role of user and data supplier are combined in one institution. This is not per se a problem as long as awareness of the role distribution is guaranteed and implications on the task assignment are taken into consideration.

Therefore, it is advised to carry out a brief inventory of the simulation team and the stakeholders and sketch out the role allocations and responsibilities. Experience has shown that, apart from specifying the responsibilities for each problem domain to be modeled and simulated, it is also advised to assign a specific person or group of persons with the tasks of integration of the domains on conceptual and implementation level and data collection and processing.

With respect to later phases of the project, especially the conceptual model design, it is also useful to assess the knowledge and competences of the simulation team concerning the components, concepts, methodologies, tools related to the system under study and domain specific M&S or M&S in general.

After the roles in the simulation team are allocated and the stakeholders identified, the actual simulation study can be started. The first phase deals with the specification of the problem and the definition of the system. According to literature this phase usually contains tasks such as:

system description, boundary definition, problem formulation, requirement specification and objective determination (see also Chapter 2.2).

Osman Balci puts great emphasis on the importance of this first part of the simulation life cycle, as the accuracy of the problem formulation greatly affects the credibility of the results. In his publications he provides detailed instructions on how to formulate a problem and subsequently derive a requirement specification [28], [38]. He defines problem formulation as *the process by which the universe of discourse is analyzed to create a formulated problem, which is sufficiently well defined to enable specific action*. He suggests the following steps to be executed in the process of problem formulation: The problem domain boundary must be established. Information and data about the problem domain must be gathered. Stakeholders must be identified and their needs and objectives must be specified. Afterwards constraints must be identified and lastly all assumptions must be specified explicitly.

The collaboration in interdisciplinary research projects has shown that an accurate problem formulation is very helpful and that the steps Balci suggests are very reasonable. Definition of the problem domain boundary deals with the question which logical and physical problem domain elements will be taken into consideration i.e. the system description. In multidisciplinary teams the system description, information and data gathering and definition of needs and stakeholders often need to be carried out in a parallel manner, since due to different level or focus of system and background information, different domain experts or stakeholders have diverging point of views on the problem domain and the nature of the problem. Therefore, it is often necessary to pass through one or more iterations, in which every domain or party first formulates its specific view of the problem and objective and then after exchange and gathering of additional information and balancing the level of information and expectations, the problem formulations are revised and should reflect a more uniform picture of the problem. This can be a very tedious process that can take several iteration to reach the desired goal, but it decreases the risk to commit the mistake of solving the wrong problem, by reflecting the formulation from different points of view.

In addition to the different points of view and knowledge backgrounds the challenge of different terminology - as mentioned in the beginning of Chapter 3 - complicates the communication between domain experts even further. In this context it has proven helpful to compile a project glossary in which project specific vocabulary or project specific use of common vocabulary is specified. This refers specifically to terms that seem to have a very clear meaning at first glance, but at closer inspection are used to describe different concepts in different domains. Examples in the context of this thesis are simulation or dynamic (see Chapter 2.1). Agreeing about a common definition of such terms within the project can help to avoid a lot of confusion.

After the definition of the objectives it is critical to assess their feasibility. If it can be confirmed, Balci suggests to proceed with a more detailed requirement definition which is based on intended uses and use cases. Intended uses refer to the purpose for which the M&S application is intended, or in other words which task it should support. This could be for instance: analysis, design identification, comparison, evaluation, prediction, selection, optimization etc. Since the intended use of an M&S application has a large impact on the requirements Balci encourages to elaborate the intended use definition into some detail. Based on the intended uses Balci suggests to specify use cases, which represent exemplary work scenarios the simulation model is required to perform in order to produce valuable results. Use cases are considered a best practice approach to handle complexity. Finally the functional and non-functional requirements can be derived from the intended uses and use cases. Overall the proposed process of the requirement definition is a very feasible one and can be recommended for the purposes of this process without many alterations. In addition it can be beneficial in some cases not only to define the intended uses, but also specify the not-intended uses. This is especially advised if there is a large number of potential (unknown) stakeholders and it is unclear whether their expectations are in accordance with the formulated objectives.

Figure 17 summarizes the process of project initialization, problem formulation and requirement definition. During the project initialization the roles within the project are specified and the knowledge, skills and competences of the simulation team are assessed. The problem formulation results from an iterative discussion process, which includes the system description, objective specification and data and information acquisition. During this phase it is also important to establish a commonly agreed terminology. The requirements of the M&S are based on the problem formulation and are derived via specification of intended uses and use cases. Adequate documentation of the results of the three main processes must be assured as well.

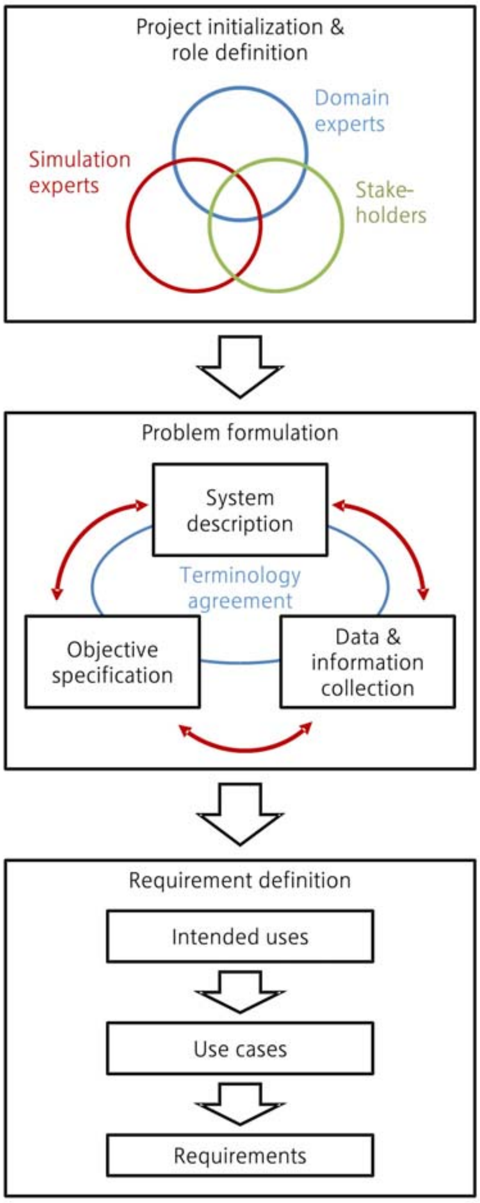

Figure 17: Project initialization, problem formulation and requirement definition process

3.3. Conceptual Model and Simulation Model

After concluding the project initialization, system description, problem and requirement formulation literature usually suggests to proceed to the conceptual modeling phase. As mentioned in the analysis of the state of the art, conceptual modeling is defined on different levels of abstraction throughout the literature (see Chapter 2.3.1), ranging from very high level generalized constructs to the actual mathematical formulation of the model.

Since this thesis is dealing with the modeling of energy flows in complex systems it will be attempted here to present a tailored conceptual modeling approach for this kind of systems that goes beyond the generic frameworks found in most publications. Based on the approaches found in literature a process to analyze the system under study and derive a conceptual model and based on it a design model, which takes the technical implementation into account, will be proposed in this chapter. The mathematical models will not be included, since a variety of parts of a system under study can be of influence to the energetic behavior and the choice of appropriate mathematical models may be equally heterogeneous. Chapter 4 will propose a mathematical modeling approach for the energy converters, distribution and storage devices. The approach described, was applied in two research projects and led to satisfying results, which are presented in Chapter 5 and 6.

The simulation life cycle process of Balci [28] from which the reference process in the previous section was derived suggests that the requirement definition is followed consecutively by the conceptual modeling, the architecting and the design. In this framework conceptual model, architecture and model design represent different levels of abstraction. The conceptual model specifies concepts and knowledge of the system of the domain under study. The architecture specification defines the fundamental organization and relationships of M&S application components. The model design specifies the models in more detail, such as mathematical modeling approaches, execution types etc. Balci suggests to use decomposition and modularization to manage the complexity of the system. Although the author emphasizes that the process is iterative the main direction of procedure is from the abstract to the specified. While Balci's approach seems very well concerted for the large M&S tasks, mainly of military background it was designed for, for the purposes of medium scale research collaborations we encountered in our projects it is less fitting.

To proceed strictly in a top-down approach implies that the conceptual model dictates the architecture, which again dictates the model design. While this enables the reuse of the more abstract concepts of the modeling life cycle, as intended by the developer [53], it inhibits the reuse of less abstract parts. For example existing model designs or even executable models cannot be reused if they are not in conformity with the architecture developed in a top-down manner. This may not be an issue with large scale simulations targeted for repeated operation over a longer period of time, where developers may be willing to design models from scratch. For smaller simulation studies that are often determined to have a very limited period of operation or number of runs, minimization of modeling effort is a concern and therefore, the reusability of existing models and domains specific simulation environments is in most cases highly desirable.

In order to satisfactorily solve the described contradiction and accomplish the highest possible degree of reusability for the conceptual model as well as the model design and executable models an alternative approach must be found. Guru and Savory identify two methodologies in the area of generic simulation: i) developing models applicable to more than one system and ii) providing libraries of model modules [51]. Therefore, they propose a modeling approach which assists in defining a conceptual model by encapsulating the information regarding the system components, arguing that the obtained model will have a reduced chance of becoming obsolete compared to executable components. Nonetheless their workflow schedules the choice of simulation tools after the development of the conceptual model.

Setavoraphan and Grant propose a conceptual modeling tool that can be applied to structure domain specific simulation environments for discrete event simulation modeling problems [54]. The authors identify a certain convergence between object-oriented approaches, often used by simulation experts, and knowledge representations from domain experts. According to the authors, the main challenge in applying object-oriented concepts and defining knowledge representations is how to determine and represent the concepts from both sides, domain and simulation experts, at the right level of abstraction. In order to overcome this barrier they suggest an approach not only based on decomposition techniques, like most literature sources suggest, but also composition techniques. The authors indicate that the reuse of results of conceptual modeling products often fails, because it has not been taken into account that reusability of models, components, modules is a challenge at abstraction level (conceptual model) but also at implementation level (simulation environments). To ensure the reusability on both levels the authors suggest to take composability into account, which they describe as *the ability to compose models/modules across a variety of application domains, levels or resolution and time scales* and *the capability to select and assemble simulation components in various combinations into simulation systems to satisfy user requirements*. There are two types of composability, which both must be taken into account: i) syntactic composability, which ensures compatible implementation details and ii) semantic composability, which guarantees a meaningful and valid composition.

Taking the above mentioned findings into account, it makes definitely sense, not to strictly proceed in a top-down manner from the abstract representation of the system under study into the direction of the executable but also to take implementation considerations into account when identifying the conceptual model; i.e. integrate a bottom-up perspective of view into the process. Therefore, an approach to take the different requirements into account is proposed here.

As suggested in most publications concerning conceptual modeling the approach fundamentally relies on the concept of decomposition. Decomposition is commonly considered a proven methodology to overcome system complexity and facilitate communication among domain and simulation experts, because the underlying concepts are familiar in many scientific disciplines and find a counterpart in the object-oriented paradigm in M&S. Furthermore, the system should be decomposed with semantic and syntactic composability in mind. Semantic composability ensures that the elements chosen to represent the system are meaningful from a system or domain point of view and the representation of their behavior and interaction is valid. This represents the top-down approach, in which coming from the system description an abstract representation of the system is formulated (the conceptual models) and is further detailed and substantiated until an executable model is derived.

During the process it must be kept in mind that the chosen decomposition has considerable impact on the model design and also the modeling effort. If the reuse of certain model elements, executable models or the application of specified simulation environments is intended, syntactic composability between these building blocks of the simulation must be assured. This must be reflected in the chosen decomposition, that must take into account that i) conceptual model element boundaries do not interfere with model interfaces, ii) every element of the decomposition can be modeled and simulated in a single simulation environment, be it domain specific or generic and iii) the necessary interfaces for exchange with other elements can be provided.

A third aspect to consider are the roles of domain and simulation experts in the modeling process and in how far these should be considered. It has been proven to be quite advantageous from an organizational point of view to have clear responsibilities for the simulation elements. In many cases, however, the implications on the conceptual model drawn from the implementation point of view and the organizational point of view show certain congruence. Figure 18 illustrates the described top-down/bottom-up approach to conceptual modeling of energy systems.

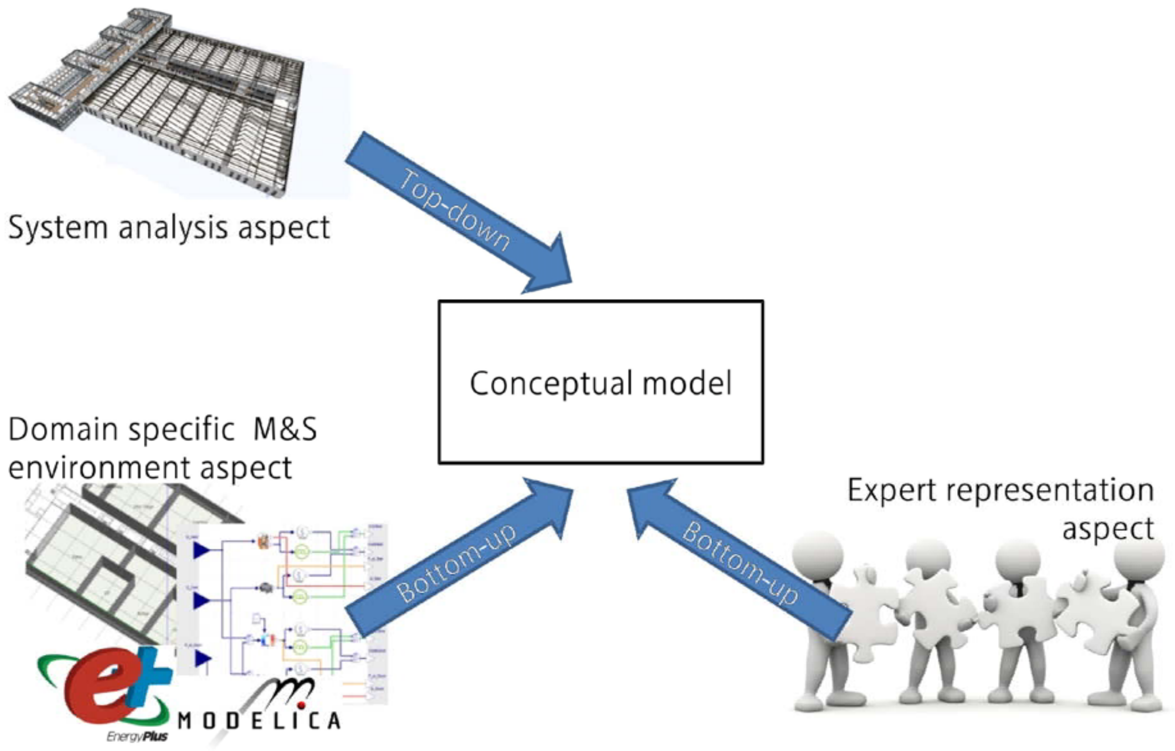

Figure 18: Top-down/bottom-up aspect integration approach to conceptual modeling

From the system point of view, while modeling a system with the objective to make a statement about its energetic behavior, the model will generally depict the part of the physical system that is related to the energy flows within the system. So the model will most likely include all components within the system boundary that use, convert, supply, distribute energy or influence the energy flows by their intrinsic behavior (user behavior, controllers...). Therefore, the conceptual model must include all the parts of the system that are considered relevant to this behavior and decompose them in manageable units. Furthermore, since energetic behavior usually evolves over time, it can safely be assumed that the core part of the simulation will conform to the definition of simulation given by Banks that states, that simulation is the imitation of a real-world process or system over time [18, p. 3]. Below more specific guidelines on how to design the conceptual model for such energy related simulation studies is suggested in terms on what to include, how to decompose and how to represent the conceptual model.

Several publications have attempted to provide guidelines concerning which elements to represent in a conceptual model. One of the early frameworks for simulation model development published in literature was Richard Nance's conical methodology, which stresses a model definition stage [48]. This stage consists of three main steps: i) model decomposition by partitioning the model into component submodels, ii) assignment of attributes to the defined objects (component submodels) and iii) classification of the attributes by type (see Chapter 2.3.1, Figure 9). Pace published a guideline which elements to include into a simulation, which is explained in more detail in Chapter 2.3.1 too [49].

Based on these generic definitions a set of objects or components and attributes will be defined to represent the system under study in the conceptual model, similar to the way Zhou et al. proposed for discrete-event simulation models [124]. The chosen structure is based on three core concepts components, parameters and variables.

First, the system is divided into components. Each component represents a coherent part of the whole system with a defined boundary towards the other parts. Therefore, the components are what Nance describes as objects and represent the submodels of the system model. As required by Pace every item specified for representation by the simulation requirements should be represented by an item and every item of potential assessment interest should be represented by a simulation element. This means that every part of the system concerned with energy flows, that are non-negligible, must be represented by a component, but it also means that components are not necessarily of a physical nature. Apart from buildings, equipment, abstract aspects like operational strategies and their economic environment may need to be described as well. If the simulation requirements call for an economic evaluation of the results implemented in the simulation, there must be a component to represent this. Further aspects of interest that may be considered as components can be data supply sources like planning activities or stakeholder interests and behavior. As required by Pace it should also be taken into account that every component has a real world counterpart, even if it is not physical. If desired, classifications of components can be introduced, such as physical components, control components, processing components, input components etc.

Furthermore Pace requires that the decomposition should correspond to accepted decomposition paradigms to ensure acceptance and effective interaction. Since the modeling tasks deal with energy systems the approach of spatial boundary specification as usually applied in thermodynamics or fluid mechanics is chosen, because it facilitates the definition of energy and mass balances. Taking the bottom-up approach into account when defining the components, it should also be assured that, for each component, at least one single specialized simulation tool exists that would cover the component in its entirety and a responsibility for the entire component can be assigned. This, however, does not imply that there can only be as many components as tools or experts are involved. Out of transparency or communication considerations a higher granularity of decomposition can make sense at this state. Of course components are of hierarchical nature. So components can be divided into subcomponents etc.

Second, after defining the components they need to be assigned attributes. The components are described by rules which determine their behavior. If the component is part of the simulation, in order to be able to build a mathematical and ultimately an executable simulation model, these rules have to be well-defined and expressed by mathematical equations. If the components represent other parts of the system, like hardware objects in-the-loop or human activities, a looser description of the behavior usually suffices for the purpose of the model. However, the description of the rules of a component is for "internal" use only. To the outside the component is exclusively represented by its interfaces i.e. to the rest of the model it is a black box. This allows combining different modeling approaches, abstraction levels and solvers or tools, and gives simulation experts the liberty to design the model according to preference.

Distinct characteristics of the components (e.g., the size of the building) are described by parameters. The values assigned to these parameters characterize a specific instance of the model. Therefore, parameters represent indicative attributes according to Nance's classification i.e. they provide knowledge about the component. In most cases they are assigned only once during a simulation execution, which makes them of permanent nature.

The current state of the components is specified by variables assigned to them. The variables are calculated from the rules and parameters and cannot be directly influenced by the simulation user (e.g. heat transferred through a wall). They represent transitional attributes according to the taxonomy of Nance.

Last but not least, the components are mutually connected and influence each other. The quantity or information characterizing this influence is an input variable for the dependent component and an output variable for the influencing one. Usually these input and output variables are only modeled if the influence is of a regular and continuous nature. Substantial but rare changes of the system (e.g., reconstruction due to management decisions) are described by a new set of parameters. The specification of corresponding output and input variables form relational attributes according to Nance. They can either be coordinated if the components are on the same level or can be hierarchical between component and its subcomponents. Since interfacing variables are explicitly specified as input or output, variable connections are directional.

When designing the conceptual model, it should also be taken into account that the rules and parameters to describe the model must have an origin. The simulation process of Banks proposes to perform model conceptualization and data collection in parallel. While it might not be possible to collect the entire set of necessary data during the conceptualization phase, keeping data availability and accessibility in mind when designing the model is advised. Sometimes parameters are derived from previous system related planning or designing activities. This results in dependencies between parameters of different components and the plan or design. In order to document these dependencies and clearly communicate the data requirements, it may be beneficial to represent these activities as elements of the conceptual model. These plan elements themselves are not part of the dynamic simulation, but define the parameterization and form a coherent point of reference in order to ensure consistency between the parameters. These dependencies are represented as parameter references between plan elements and simulation components.

As mentioned previously the model will generally depict the part of the physical system that is related to the energy flows within the system. So the model will most likely include all components within the system boundary that use, convert, supply, distribute energy or influence the energy flows by their intrinsic behavior (user behavior, energy consuming equipment, controllers, etc.) and other components to represent influences, processing of simulation results etc. Upon deciding on what to include into the model and where to locate the component boundaries and how to interface the components, a non-exclusive list of questions may provide some guidance.

Decomposition according to a system related point of view (top-down):

- Which parts of the system require energy, supply energy, or in some way modify, convert or distribute energy?
- Which strategies and controls are needed to steer the physical parts related to energy?
- Where do energy flows move? Can all the energy flows be calculated at the system boundary (criteria for thermodynamic balances)? Is a simplification to causality possible?
- Where do mass flows move? Which mass flows are energy relevant i.e. transport energy? Can all mass flows at the system boundary be determined?
- Which control and steering variables are relevant to the control of the energy flows?
- Which information flows are furthermore required i.e. because they trigger energy flows (temperatures in other components that provoke heat flows), provide feedback for controllers.
- Which external influences or disturbances influence the system?
- Which information about the system must be gathered?

Decomposition according to design and domain related points of view (bottom-up):

- Is there at least one single specialized simulation tool that would cover the component in its entirety?
- Can one person take the responsibility for the component in its entirety?
- Are there any non-simulation parts to be considered (in-the-loop)?
- What does the front- and back end of the simulation look like? Are there any elements for parameter supply needed? Are any simulation data post processing component required?

It must also be mentioned at this point that the modeling procedure of decomposition at this level is a purely deductive approach to modeling, because the processes rely on understanding the physical and informational interdependencies between system parts. Therefore, the top-level conceptual model is a white box model. The components are, from the perspective of the top-level conceptual model, black box models, because only the inputs and outputs are known. If the model inside of the component results from deductive or inductive approaches or a mixture of both, is of no consequence to the higher level model.

3.4. Documentation and Validation

After the specification of the components and their attributes, the defined model must be documented in a suitable manner. Often graphical representations are chosen to document models. According to Kop and Mayr there are several reasons, why graphical modeling languages are popular [47]. According to them the two main advantages are that humans are visual beings and that graphical representations provide a spatial overview and overall description of the problem and offer an excellent summary. But they also identify drawbacks of the concept. First of all the reader must be familiar with the semantics of the used symbols and second too large or complex systems become confusing for the beholder. Graphical representations fail, because they overwhelm the reader if a large number of objects and too many different kinds of notions, described by different symbols, is assembled. Therefore, dealing with complex systems, the information provided in graphical representations is usually incomplete. Much like an iceberg, the majority of the information is hidden beneath the surface.

Taking these considerations into account a combination of a graphical representation and a template based description is proposed in order to document the conceptual model. Experience in application has shown that representing the top level components, elements and relational attributes (variable connections and parameter references) in a graphical manner is a very helpful base for discussion among experts and usually the size and complexity stays within limits. All the other information can be documented in textual form.

The components and plan elements should be represented as spatial objects (squares, ovals...) and it should be assured that plan elements and components, or different kinds of components, if such were defined, are visually distinguishable. All components and elements should be characterized with a unique name and/or acronym. Variable interfaces and parameter references can be represented be arrows since they are directional. Representing every single variable or parameter may again be too much information for the graphical representation. Therefore, it is advised to collect all variables or parameters with the same origin and destination in one arrow, characterized by a unique identifier (e.g. output component-input component), and list the variables in the textual description. Again variable interfaces and parameter references should appear in a different shape or color. Figure 19 shows an example for the graphical representation of a conceptual model.

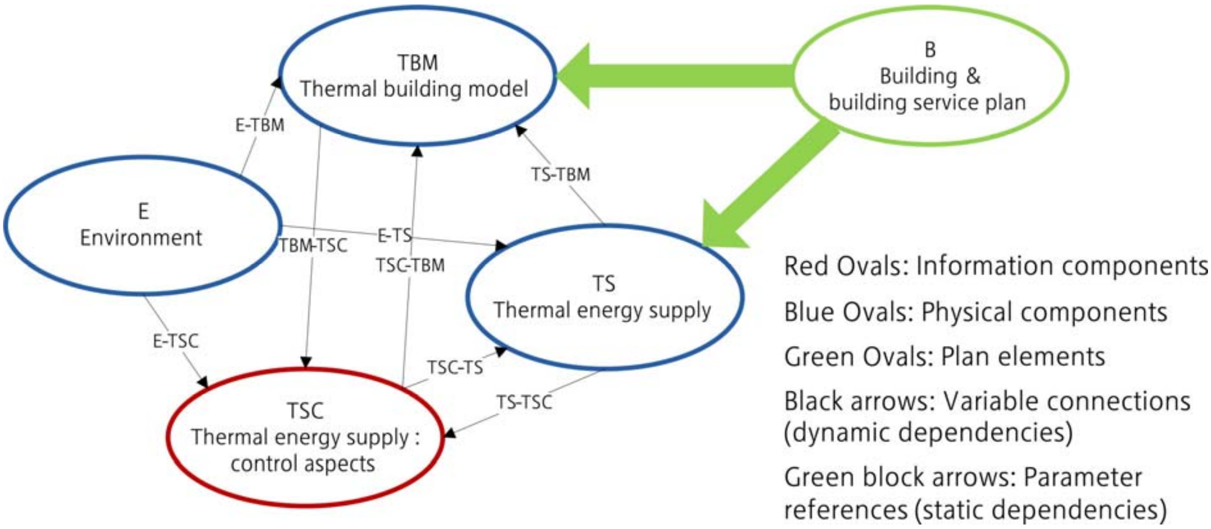

Figure 19: Example for a graphical representation of a conceptual model

Apart from the graphical representation the conceptual model should be represented in a textual manner in order to document the model in its entirety. The documentation should consist of two parts: a general description of the whole model and component specific parts. The general description of the model should contain the specifications of the initialization phase, problem formulation and the requirement definition. Furthermore, and overview of the components and elements should be given and if any further distinctions between types of components are being made this have to be documented as well.

The component specific part should be equally structured for all the components. For the purpose of structuring model specific information template based representations of conceptual models have been proposed in literature [42], [51] and a similar approach shall be chosen here. Table 1 provides an example for a component template developed in the research project INFO. The interfaces between the components aren't defined in both, the in- and output component, but only in one, in order to the reduce risk of incompatibility and maintenance effort. It was chosen to specify the interfaces on the side of the input component, with the hope that the responsible person on the receiving end has more interest in keeping the specification updated than the one on the providing end. The proposed template is of course to be seen as a suggestion and can be modified according to demand. In some cases it may be helpful to provide more information (e.g. about the mathematical model) or a less detailed definition is sufficient to meet the demands of the M&S task.

Table 1: Component specification template

Component identifier		
Component name		
Component type		
Executive summary		
One sentence description of the component		
Component description		
Narrative description of the system part that is represented by the described component, descriptions of the abstractions and assumptions made and if applicable the chosen modeling approaches		
Interface description		
Narrative description of the interfaces of the component (input and output), the relations to other components and the abstractions and assumptions		
Parameters		
	Parameter name	*Phys. unit*
	…	
Input Variables		
	Origin component	
	Variable name	*Phys. unit*
	…	
	Origin component	
	Variable name	*Phys. unit*
	…	

After carefully documenting the conceptual model, a simulation model which represents the transition from the conceptual model to the implementation can be derived from the conceptual model. The simulation model describes the allocation of the components of the conceptual model to certain simulation engines or hardware components. Since the conceptual model was already designed with the aspect in mind that every component could be executed by one single simulation environment, this task simply consists of uniting conceptual model components to simulation components and reducing the conceptual model interfaces to the interfaces that must be implemented (see Figure 20).

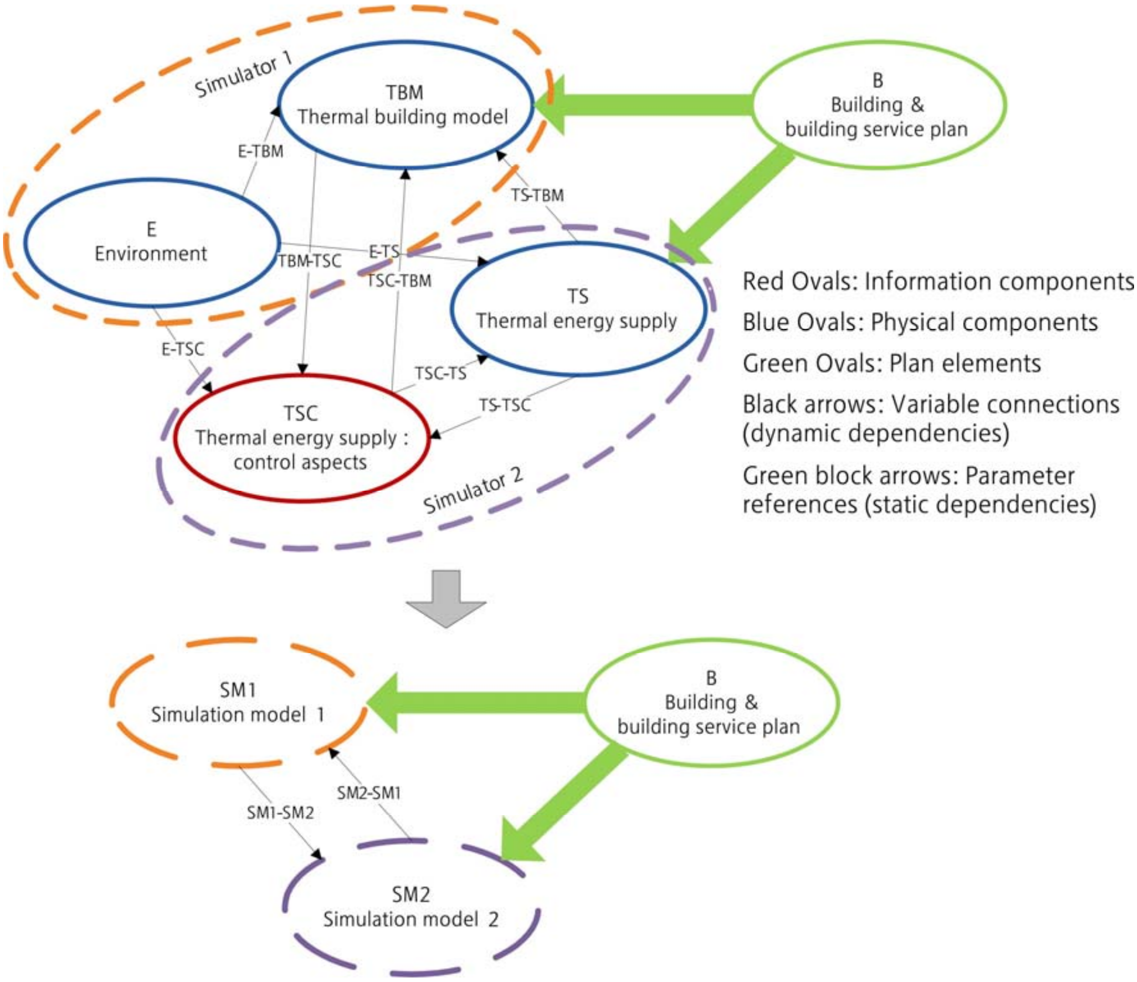

Figure 20: Reduction from conceptual model to simulation model

In addition to the specification of the interfaces in terms of the variables to be exchanged the temporal aspect must also been given some consideration. In case of continuous simulator runs the exchange intervals must be specified. In case of a discontinuous run or in-the-loop applications the points in time, at which the coordinating simulator is paused and the external simulators are called, must be specified. Furthermore, the temporal parameters of each simulator must be defined (simulation time, times step). Chapter 6 provides an exemplary visualization of the temporal organization of a discontinuous hardware-in-the-loop simulation.

As mentioned in Chapter 2.2 most literature about modeling and simulation processes suggests that the whole modeling process and the simulation execution should be accompanied by appropriate validation and verification (V&V) processes [18], [27]. Balci goes as far as to require accompanying quality assurance processes for the whole simulation life cycle; starting from the problem formulation until presentation of the results [28]. Therefore, the processes leading from the project initialization to the conceptual model should be accompanied by according measures. Since in the first stages of the development, results are often not very concrete, formal validation techniques are most often not applicable. However, a number of informal validation techniques can be applied to ensure the quality of the obtained results. Balci and his colleagues have published a number of papers concerning the right validation and verification techniques for each stage of the modeling and simulation process [32], [33], [37]. For the first stages of the modeling process he suggests mainly the following techniques:

- Desk Checking is the most commonly used V&V technique, which is simply reviewing one's work in terms of logic, consistency and completeness. However, desk checking should not be applied after testing a model, in order to determine, why it does not work, but in advance and preferably not by the modeler
- Documentation Checking is essentially the same as desk checking but not concerning the model but the documentation.
- Face Validation involves individuals in possession of in depth system knowledge, who are asked whether they deem the logic of the model structure correct and the input - output relationships reasonable. [27]
- Walkthroughs are a more formal approach to V&V then checking and face validation. They have the same purpose as checking techniques do, i.e. examining the models structure and character in detail, but are an organized activity, following certain guidelines. Walkthroughs are performed in teams, which analyzes the model in terms of consistency and completeness.
- Inspections are a more formalized alternative to walkthroughs. Particular roles are assigned to the inspection team members (moderator, designer, implementer, tester) and a chronological sequence of phases are performed (overview, preparation, inspection, rework, follow-up).
- Reviews are similar to inspections from the procedural point of view, but their goal is not to ensure model validity. They are intended to give the model stakeholders feedback if the development process is proceeding according to the defined objectives.
- Audits seek to determine the adequacy of the development process with respect to guidelines, standards, practices.

All the mentioned techniques, apart from the latter two, aim at ensuring the consistency and completeness of the model with the physical system. It generally seems like a good idea to concentrate on validating the logical and structural validity of the model at this point. Since the model was derived from the system understanding or knowledge about the system in a deductive manner it must be assured that this was translated into a valid model. Furthermore, to this point the model has not produced any results that could be compared to known data about the system. Therefore, the only potential source of information to compare the model to is mental knowledge about the system. Although the use of mental knowledge provided by domain experts as reference information for validation is sometimes considered questionable, many researchers have accepted this approach as practicable alternative if other data is lacking [27], [35]. The above presented techniques provide structured procedures to perform knowledge based validation. In this context also the importance of the graphical representation of the conceptual model cannot be underestimated, since graphical models are considered extremely helpful tools for model validation [31]. Furthermore, it must be taken into account, that not only the top-level conceptual model must be validated but also potential submodels. Popper provides an extension to Sargent's simulation cycle taking the submodel validation into account [22, p. 52].

Input data validity is not a concern up to this point, because apart from structural and behavioral information, little data was used in the modeling process so far. And the correct transfer of this information is covered by the above mentioned procedures. Apart from validity with regards to content, it is important to ensuring compliance of the model with the objectives and requirements of the simulation study. Review and auditing techniques provide the appropriate tools to conquer this task.

Another important aspect to take into account when designing the validation process is the role allocation. Simulation team members, stakeholders and also third parties can be involved into the validation process. Sargent has given this topic some thought and concluded that if the simulation team is small, it is preferable to involve users or third parties in deciding the validity of the model [27]. However, if the simulation team is of sufficient size "cross-validating" between domains can be an option.

Due to the rather abstract nature of the conceptual model the validation process is equally so. Diving deeper into the domain models of the energy system in Chapter 4 and the results of the M&S simulation processes in Chapter 5 and 6 more ideas about computational model verification, operational validation and data validity will be discussed.

4. Energy System Model Library

The previous chapter described the decomposition of the system into a conceptual model on top-level. This chapter will go into more detail about the realization of the energy system models and also briefly suggests an approach to thermal building modeling. The considerations are limited to energy systems only, because the modeling approaches chosen for other aspects of the system are highly dependent on the nature of the systems and the domain specific modeling traditions. Narrowing the modeling domain, the chosen modeling paradigms and their implications on validation, verification and implementation are discussed in more detail. Mathematical models for a model library, designed according to the discussed consideration and including the most commonly used energy system components, are presented.

4.1. General Considerations Concerning Model Design

The model of the energy system depicts all devices that ensure the useful energy supply of energy users within a system, any form of equipment, the building itself and auxiliary devices. Most commonly the system receives final energy from the energy supplier (electricity, gas, heat etc.) or primary energy from the environment (solar irradiation, geothermal heat etc.) and supplies different forms of useful energy: thermal energy, electric energy and other forms, such as mechanical or chemical energy.

The thermal energy supply describes all facilities supplying thermal energy (transformation, storage, distribution and injection). This includes heating, cooling and air conditioning of the building, warm water supply, cooling of machines and central IT devices and process heat and cold. Complementary, the non-thermal energy supply includes likewise externally provided energy (from the grid), energy recovery, in-house production and storage, as well as distribution systems. Potential energy sources are mainly electricity (grid, photovoltaic, wind power), gas (fossil fuels and biogas), biomass, and possibly other sources, such as mechanical energy (pumped storage).

The distinction between thermal energy supply and the other energy forms is of interest for the modeling approach for two reasons. Firstly the transport of thermal energy is in most cases tied to the mass flow of the heat transfer fluid (HTF) and secondly the exergy content is not dictated by the form of energy, as it is the case with electrical or chemical energy, but depends on the state of the heat transfer fluid.

In addition to the energy conversion systems the energy system model includes the control of these systems.

In general the described energy systems rely on a number of different types of machines and components that are assembled into systems in a multitude of different ways, in order to respect the system peculiarities. This leads to the consequence that certainly one model cannot cover all the possible system configurations. Hence, if reuse of the developed model components is intended, other strategies are called for. Balci et al. suggest that the reuse of model components, even if they are not executable components, enables the faster and more efficient assembly of models [53]. Guru and Savory propose the extension of this approach to executable models in order to provide simulation module libraries. According to them, libraries and models that are applicable to more than one system are the only two methodologies to accomplish generic simulation [51]. Setavoraphan and Grant identified three techniques to achieve reusable models [54]: Assembly enables connecting existing model components through a common environment. Extension allows modifying the functionality of a model component by selective activation of features. Parameterization offers adaptability of the operational and behavioral characteristics of model components. All this suggests that the most feasible approach to design the models for energy systems is a component library, whose modules can be assembled in order to mirror system characteristics and can be modified by parameters and extensions in order to reflect specific instances of the component.

Concerning the modeling approaches of primary and secondary energy system components Marija Trčka makes some interesting observations. Primary systems are energy converters, while secondary systems summarize systems for fluid distribution. Distribution components should always satisfy energy and mass balance i.e. they are described by physically models in most BPS tools although mostly in a simplified way. Energy conversion components, due to their technical complexity mostly rely on empirically obtained equations, using inputs from test data or manufacturer supplied design data. [45]

The trend to apply deductive modeling techniques at the level of system assembly and inductive techniques at component level, certainly offers a few advantages. In a deductive modeling process the mathematical model is derived analytically by using knowledge of the structure of the system, the underlying (physical) laws and parameters. Due to the nature of deduction a model constructed this way presents a unique solution of the modeling problem. This perfectly corresponds with the nature of energy systems, whose configuration is mostly well known and which are usually quite unique in realization. On the other hand an infinite number of inductive models can satisfy a given data set, which is the perfect basis for modeling different forms of the same component type with one model, by modifying the parameterization.

The inductive approach also satisfies the requirement to be able to parameterize the components easily on the basis of readily available manufacturer data or test results which are usually none other than input – output relations. Complex physical models, for which detailed constructional data is needed, would not satisfy these requirements. Additionally, inductively derived models are usually simpler than deductive ones, which carries, according to Stewart Robinson, several advantages: faster development, more flexibility, easier interpretation of results, faster simulation speed and less data requirement, which also reduces the risk of decreased accuracy due to data insufficiencies [42].

Under consideration of the above mentioned aspects of simplicity, flexibility and data availability for parameterization models based on characteristics and simplified physical models were used to comprise the model library. For energy converters the model input is in many cases defined as the required power and the output as the power demand or the fuel consumption required for providing the demand. The model structure of such an energy converter model is shown in Figure 21.

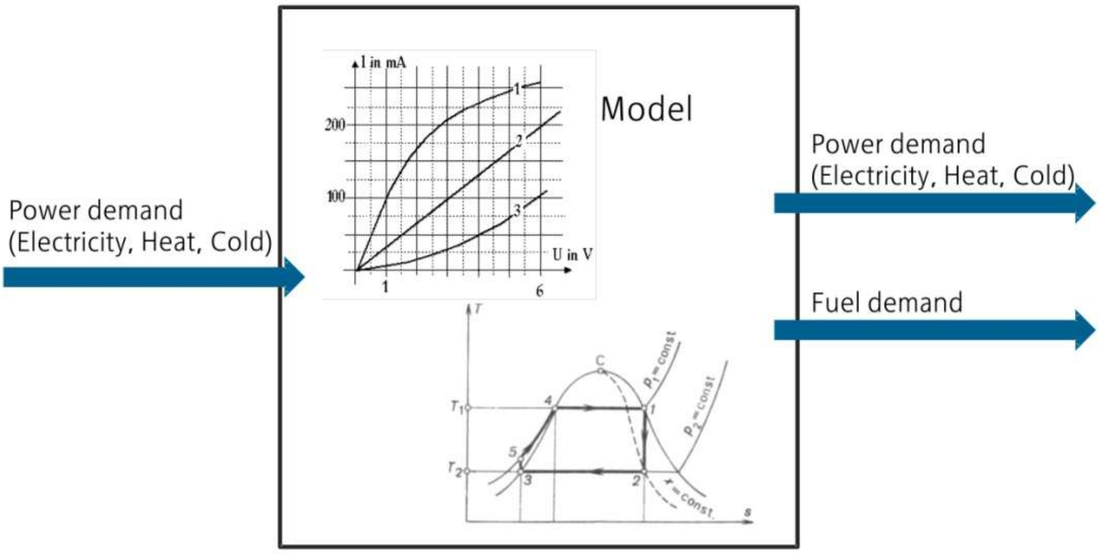

Figure 21: Model architecture for energy converter component models

Simplifying the calculation of energy and mass balances in the secondary systems also makes sense. As mentioned above, most directed heat flows in building systems are transported via heat transfer fluids and therefore expressed by the state variables of the HTF. Mapping of energy transport by calculating the mass flow of the HTF in the hydraulic system requires not only the calculation of the state variables at every point of interest but also the calculation of the pressure drop which triggers a mass flow. The entire hydraulic system (pipes, valves, etc.) must be known in detail and modeled entirely. This poses a source of problems for reasons of data availability and computational effort. Therefore, in the most cases it makes more sense to forgo this acausal modeling approach and represent the distribution systems in a simplified way as energy balances around system nodes and heat flows by the power transferred between them, which eliminates the need to calculate the pressure drop. This however, also results in the loss of the state variables of the heat transfer fluid. Mostly this is not considered a problem since most supply and return lines are operated on fixed temperature/pressure levels either exclusively in liquid or gaseous state of aggregate. In that case the states can be treated as a system parameter. Otherwise, the system nodes where the state is of interest can be realized as a dynamic component and one state variable can be calculated by using the energy balance, if the others are known.

Although some simplifications are applied to the modeling of the energy distribution systems, a modular structure that enables the reuse of certain components makes little sense on this level, since, as mentioned above, in most cases energy systems are unique solutions. Therefore, assembling and correctly linking the components must be done for every instance of the model from scratch. The same applies for the underlying control, which is in most cases a coordinated solution for the respective system and equally unique.

By applying these principles to build a model library and leaving the arrangement of the components to a system model to the modeler of the instance, the requirements of assembly, extension and parameterization are fulfilled and flexible and reusable systems can be created.

4.2. Validation and Verification

Chapter 2.2 lists a number of validation techniques, suggested by literature [32], [33], [37] for conceptual models. Since in the stages of conceptual modeling simulation results are unavailable, formal validation techniques are most often not applicable. Therefore, the suggested validation techniques are mainly dependent on expert knowledge and rely on more or less structured checking of the models in terms of logic, consistency and completeness or concerning conformance with the objectives and quality standards. Validation of the energy system conceptual models and also mathematical models can and should be executed following the same techniques and standards as the top level conceptual model. Additionally, as with the top-level model, careful consideration of the role allocation is advised. Robert Sargent suggests that it is preferable to let users or third parties decide the validity of the model rather than the M&S team itself [27]. When only a part of the simulation team is involved in the creation of a sub-model, other members of the team can take on the role of a stakeholder. Therefore, they can be tasked with deciding the validity without violating Sargent's claim.

After validation of the conceptual and mathematical model, implementation produces an executable model from the specifications. Verification deals with the question, whether the model was correctly implemented. For verification Whitner and Balci suggest, apart from close inspection of the code using the same informal methods as for validation, a number of analysis and testing methods [33] an overview of which is given in Figure 22.

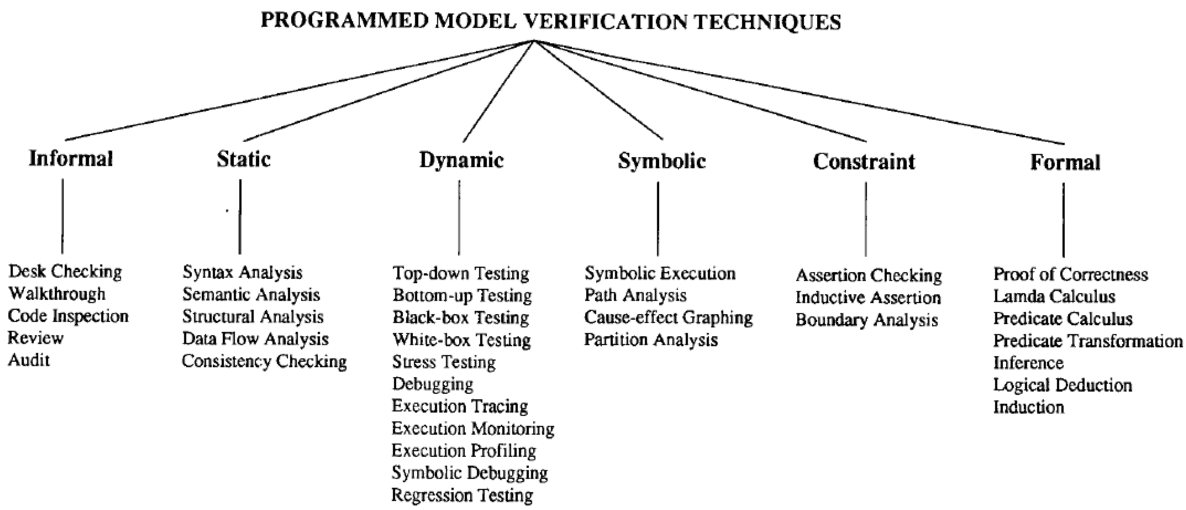

Figure 22: Taxonomy of programmed model verification techniques by Whitner and Balci [33]

Static analysis is concerned with verifying the static model source code. It does not require model execution. The most minimal form of static analysis, determining the syntactic correctness, is to successfully compile the model. The other forms of static analysis deal with the question if the executable model correctly reflects the conceptual model and apply different techniques to ensure it. Dynamic verification requires the execution of the model and includes several testing techniques, based on the information gathered during execution. It is important that the testing techniques must correspond with the modeling techniques. Some of the above mentioned strategies can be applied for verification of the energy system model; some are more suitable for models following other model paradigms. If a model is implemented top level first, is makes sense to start testing at top-level. If submodels are designed first and integrated later starting the testing with the submodels makes sense. The same applies to black- and white-models and testing techniques. Since the design of the energy system model mainly consists of bottom-up techniques (components first, than interfacing them) an according testing strategy is advised. Since most component models are executed as inductive models it also makes sense to test them by applying comparing input-output relationships rather than examining the inner logics. For the V&V of the integration of the energy system components to the overall energy system of course the opposite is true. Since the internal laws are known white box testing can be applied. The same is true for the top-level system model, which should also be tested in a top-down manner. Furthermore, close execution monitoring of simulation execution events and tracing of system variables can be helpful. Another feasible technique, especially if input data is not yet available, is symbolic execution, where actual data values are replaced by symbolic values, based on which the outputs are determined. A big advantage of symbolic execution is that it shows path correctness for the computation regardless of test data. Assertion checking comes in very handy to determine whether assembled models actually perform according to their specification i.e. as the modeler assumes they do. Assertion statements which compare the assumed values for certain variables with the calculated values are implemented into the model code and can be conveniently reviewed by the modeler.

All the component models presented in 4.4 were subjected to static analysis in terms of semantic analysis, consistency checking and of course syntactic analysis by compilation. Furthermore, symbolic executions were performed with all of them. If useful parameterization, input and output data for comparison could be found (e.g. from manufacturer data) black box tests were executed.

Figure 23 and Figure 24 show the comparison of simulation results with results for operation scenarios calculated manually, based upon data provided by a manufacturer of absorption chillers. Since the input data and parameterization were the same, results show a good resemblance, which verifies the model to a large extent.

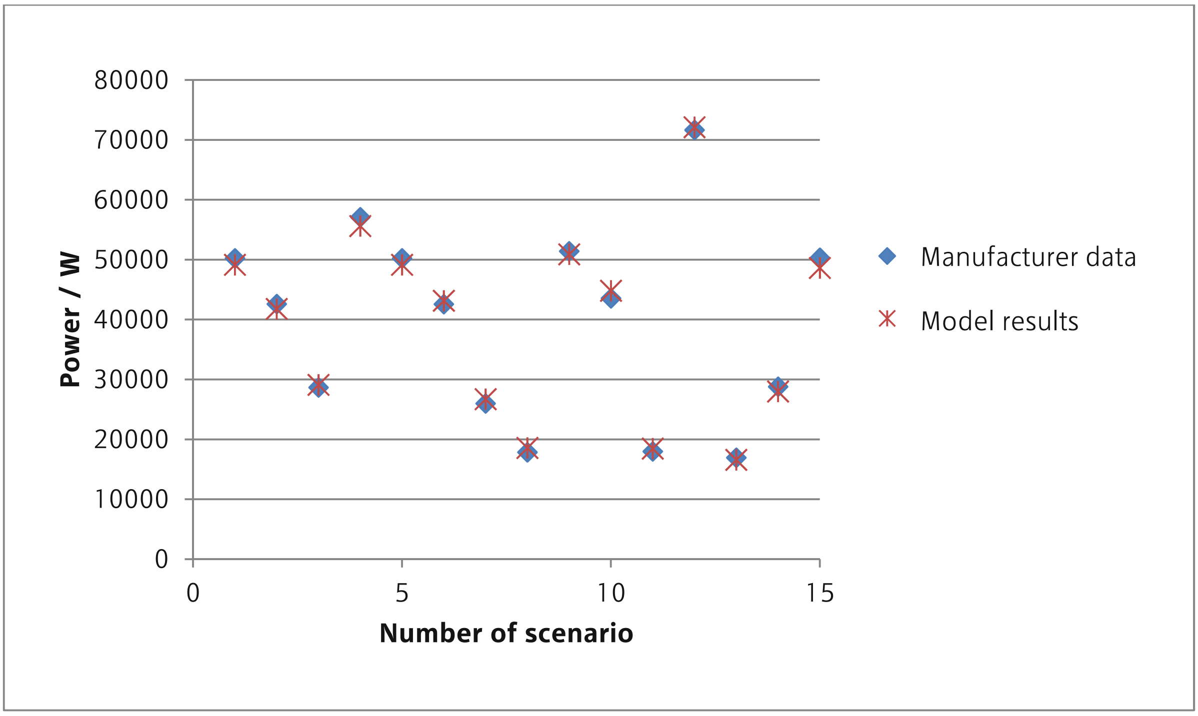

Figure 23: Verification of absorption chiller model, comparison of consumed heating power [125, p. 62]

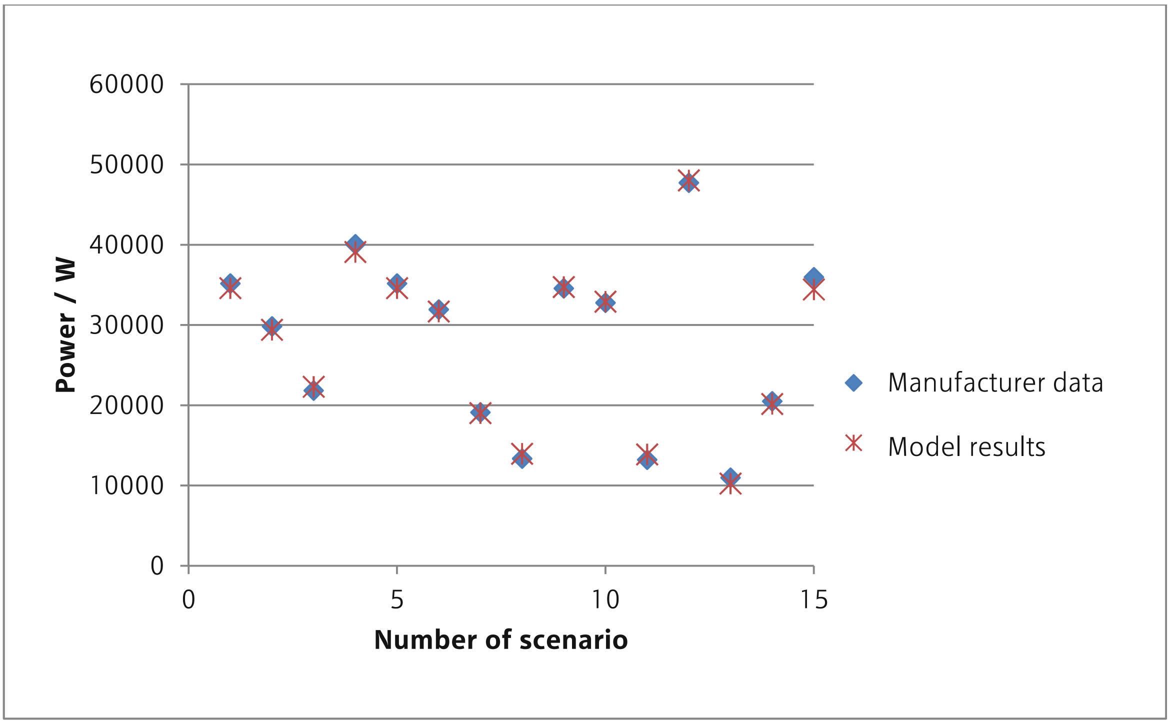

Figure 24: Verification of absorption chiller model, comparison of supplied cold [125, p. 62]

However, the test does not make a statement about the validity of the input data, it merely determines that the manufacturers specifications about the chiller can be replicated correctly by the model. Since the underlying model is a mainly inductive model that does not proof much, because determining the correct input/output relation by interpolation from a field of characteristics is not a groundbreaking modeling accomplishment. The real question that determines whether operational validity is given in this case i.e. that the model outcome is of sufficient accuracy for the intended purpose [27], lies in the data quality. In case the modeled absorption chiller is not actually in operation yet, the results cannot be compared with measurement data and we must believe that the manufacturer data represents the actual behavior of the machine under real-world operating conditions, which can sometimes be doubtful. This aspect represents a real drawback, because the combination of a quite-black box model, which already has a lower expected validity factor according to Karplus [59] (see also Chapter 2.3.2) and doubtful data validity severely affect the operational validity and therefore the credibility of the model.

According to Sargent operational validity can only be assured by comparing simulation results to real system [27]. So if the real system does not exist or is somehow inaccessible as a data source and no other model can be used for comparison, the model results should be considered rather as qualitative indicators then quantitatively precise predictions. A sensitivity analysis could determine the impact of flawed data of singular components on the overall system behavior.

4.3. Implementation Considerations

Based on the general considerations about the model design and the additional claims by the integration into complex simulations certain requirements for the model implementation can be extracted for selecting the used simulation tools.

In order to guarantee the interoperability with other models, the use of a simulation environment, which facilitates the coupling, is advisable. Some simulation environments such as

Matlab, Dymola and TRNSYS offer interfaces for facilitated coupling with other simulation environments and co-simulation frameworks such as BCVTB (see Chapter 2.5).

Following the described library structure, in which a wide range of components that can be used in different configurations for assembling the overall energy system, an environment which allows implementing a modular system should be used. This requires the modeling environment to follow object-oriented modeling paradigms.

Due to the need to newly model the rules for the system assembly and the control for every system instances and the differences in the description of the components used (data sheets of machines of the same type do not always list the same parameters for characterization) emphasis should be put on facile model adaptability when choosing a suitable programming environment. Use of a higher modeling language can significantly facilitate this task.

Based on the above mentioned requirements the modeling standard and simulation tool of choice for the implementation of the library turned out to be Modelica and Dymola, respectively.

Modelica is a C++ based modeling standard and offers an object oriented modeling language for physical modeling as well as commercially or freely available model libraries. The Modelica standard library offers classes for all basic mathematical operations (unit definition, functions,...) which can be reused for subclasses by means of inheritance. Furthermore, the standard library defines components for modeling of mechanical, electrical, thermal und hydraulic phenomena. Basic components (e.g. resistors, inductance, and capacities for electrical systems) are provided and can be connected by so called connectors, which operate using acausal Bond-Graph logic. Additionally components can be linked causally via in- and outputs signal, thus using a directional signal flow. Applying this approach the library offers a selection of logical and signal processing components as well as simple control units. Aside from the standard library an encompassing selection of free and commercial libraries for specific applications is offered for the Modelica standard.

As mentioned above, using acausal modeling approaches are not advised to model energy transport in HTFs. Therefore, the acausal connectors provided by Modelica were not used, but the component connections were reduced to causal signal flows.

4.4. Energy Systems Model Library

As mentioned in section 4.1 the energy system to be depicted in the system models consists of primary and secondary systems. Primary systems are energy converters, secondary systems are systems for energy distribution.

4.4.1. Primary Systems

Concerning primary systems the most typical energy conversion systems found at energy users sites should be integrated into the library. Table 2 gives an overview of the energy conversion system models integrated into the library, classified by supplied and produced form of energy.

Table 2: Overview of energy conversion models in library

Production / *Supply*	Electricity	Heat	Cold
Solar Energy	Photovoltaic (PV)	Solarthermal collector	
Wind	Windengine		
Electricity		Resistance heater	Compression chiller
Electricity and heat at low temperature		Heat pump (from waste heat, well, soil)	Cooling tower
Heat at high temperature (>75°C)		Direct use	Absorption chiller Adsorption chiller
Heat at low temperature		Direct use (from waste heat, geothermal heat exchangers)	
Cold			Direct use (from well, river, soil)
Biomass	Biomass combined heat and power (CHP) Biogas CHP		
		Biomass boiler	
Fossiles (Gas, Oil, coal, ...)	Gas CHP / Oil CHP		
		Various Boilers	

As described previously the basic structure of the models for these energy conversion systems are based on characteristics that relate in- and outputs. Furthermore, simplified physical relations are added, usually derived from the first or second law of thermodynamics, in order to calculate outputs not determined by the characteristics. If the energy conversion component supplies upon demand the model input is in most cases defined as the required power, the output the power demand or the fuel consumption, required for providing the demand, is calculated. If the component produces whenever supply is granted (e.g. a photovoltaic system) the supply acts as an input and the production is the output. Additional in- and outputs such as ambient conditions or states of media can be necessary if they are determining for the component's operating efficiency.

Dietrich Wertz proposed modeling approaches for several types of energy converters in his PhD thesis [121], some of which fulfill the above mentioned model requirements and could be reused for the model library after some adjustments of interfaces. The models for the photovoltaic systems, solar thermal collector and wind engines were integrated and shall be described briefly. A more detailed description can be found in Wertz's thesis.

Component Model: Solar Thermal Collector

In Wertz's solar collector model the conveyed heat flow is calculated based on an energy balance. One part of the supplied power, which results from the incident solar radiation minus all losses due to reflection, conduction and convection, is expended for warming up the thermal mass of the collector and the other part is conducted by the collector fluid. This leads to the pivotal equation:

$$k_\Theta\, \eta_{coll}\, I_{coll_{tot}}\, A_{coll} = \frac{C_{p\,coll}}{2}\left(\frac{d}{dt}T_{SL} + \frac{d}{dt}T_{RL}\right) + \dot{m}\, c_{p_{HTF}}\,(T_{SL} - T_{RL}) \tag{4}$$

In order to describe the collector's properties, the collector efficiency η_{coll} and the angular factor k_θ are introduced. The latter describes reflection and absorption losses dependent on the angel of incidence of the solar radiation θ_{coll} and can be calculated by using the collector's characteristic values b_0 and b_1:

$$k_\Theta = \left[1 - b_0\left(\frac{1}{\cos\theta_{coll}} - 1\right) - b_1\left(\frac{1}{\cos\theta_{coll}} - 1\right)^2\right] \tag{5}$$

In case only the angle factor for 50° incidence angle $K_1(50°)$ is available, the quadratic term is neglected ($b_1 = 0$) and b_0 is calculated as:

$$b_0 = \frac{1 - K_1(50°)}{\frac{1}{\cos(50°)} - 1} \tag{6}$$

The collector efficiency η_{coll} at a certain operating point can be derived from the collector characteristics, which is approximated by equation (7) using three characteristic values: collector conversion factor c_0 (efficiency at $T_{amb} = T_{coll}$) and the linear and quadratic heat loss coefficients c_1 and c_2.

$$\eta_{coll} = \left[c_0 - c_1\frac{T_{coll} - T_{amb}}{I_{coll_{tot}}} - c_2\frac{(T_{coll} - T_{amb})^2}{I_{coll_{tot}}}\right] \tag{7}$$

$$\text{with } T_{coll} = \frac{T_{SL}+T_{RL}}{2} \tag{8}$$

In order to integrate the model into the library the interfaces were adapted to fit the above mentioned concept. The model follows the pattern supply as an input (I_{coll_tot}) and production $\dot{Q}_{out} = \dot{m}\, c_{p\_HTF}(T_{SL} - T_{RL})$ as an output. But the model furthermore needs the return line fluid temperature T_{RL} in order to be fully determined, illustrating the state variable problem described in Chapter 4.1. The temperature can be set as a parameter, if the system operates with fixed line temperatures, which is usually not the case for solar thermal systems, because the return line temperature is determined by the storage temperature. Therefore, the temperature must be supplied as an input by the grid model, which in order to provide this information, must calculate a temperature as dynamic state variable (e.g. the lowest storage temperature). Furthermore, an interface for a control variable, turning the system on and off, depending on the relation between the supply line temperature and a certain reference temperature, must be implemented.

Component Model: Photovoltaic Collector

Dietrich Wertz's model for the photovoltaic collector calculates the output power as a function of irradiance (I_{coll_tot}), nominal efficiency (η_{PV}), angular factor (k_θ), pollution factor (k_D) and module temperature factor (k_T).

$$P_{el} = I_{coll_{tot}}\, A_{coll}\, \eta_{PV}\, k_\theta\, k_D\, k_T \tag{9}$$

The angular factor is calculated according to equation (5) and (6). The decrease of efficiency caused by the collector temperature is determined as

$$k_T = 1 + c_T\,(\vartheta_{coll} - 25°C) \tag{10}$$

with c_T ranging from $-0{,}0018\ 1/\mathrm{K}$ to $-0{,}005\ 1/\mathrm{K}$ according to the type of PV cells. The collector temperature is calculated using the same balance as for the solar thermal collector. If the PV is not cooled the balance the outgoing heat flow is set to zero: $\dot{Q}_{out} = \dot{m}\, c_{p_{HTF}}\,(T_{SL} - T_{RL}) = 0$.

Component Model: Wind Engine

In order to calculate the power in dependency of the wind velocity u Wertz used the linearized characteristics of a wind engine. Below a defined start-up velocity no power is derived. Above it the output power increases linearly with the wind velocity until reaching the nominal power of the engine and remains at this value even when further increasing wind velocity. If the wind velocity increases beyond a certain cut-out velocity, the turbine is turned off for safety reasons and the power becomes zero.

$$P_{el} = \begin{cases} 0 & for\ \ u < v_{start-up} \\ \dfrac{u - v_{nom}}{v_{nom} - v_{start-up}} P_{nom} & for\ v_{start-up} \le u < v_{nom} \\ P_{nom} & for\ v_{nom} \le u < v_{cut-out} \\ 0 & v_{cut-out} \le u \end{cases} \tag{11}$$

Component Model: Absorption Chiller

The absorption chiller model, which was created within a bachelor thesis by Tobias Smuda [125], calculates the three heat flows linked to the mass flow rates of the heating, cold water and cooling water, the delivered cooling power and the absorbed heating power and the COP. This model interpolates from several sets of characteristic curves as the machine performance depends on several degrees of freedom.

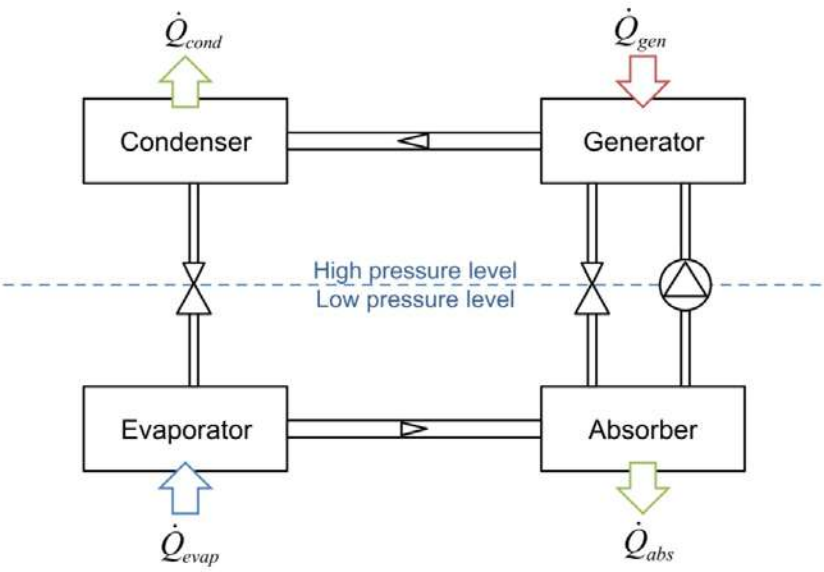

Figure 25: Heat flows in and out of an absorption chiller according to [125, p. 24]

The delivered cooling power as well as the absorbed heating power change with cooling or heating water inlet temperatures $(T_{cool_{in}}, T_{heat_{in}})$ deviating from nominal conditions. These influences are considered by introducing two correction factors: the cooling capacity factor CCF and the heat input factor HIF which are both functions of the cooling or heating water inlet temperatures $T_{cool_{in}}, T_{heat_{in}}$. The heat medium flow correction $HMFC(\dot{m}_{heat})$ incorporates the effect of the heating water mass flow $(\dot{m}_{heat})$ deviating from nominal conditions. This effect can be used to realize a certain amount of part load operation by throttling the mass flow.

The delivered cold $\dot{Q}_{evap}$ and the absorbed heat needed to separate working fluid and solvent in the generator $\dot{Q}_{gen}$ result from:

$$\dot{Q}_{evap} = CCF\left(T_{cool_{in}}, T_{heat_{in}}\right)\ HMFC(\dot{m}_{heat})\ \dot{Q}_{evap_{nom}} \tag{12}$$

$$\dot{Q}_{gen} = HIF\left(T_{cool_{in}}, T_{heat_{in}}\right)\ HMFC(\dot{m}_{heat})\ \dot{Q}_{gen_{nom}} \tag{13}$$

The exported cooling water heat flow $\dot{Q}_{cool}$ produced in the condenser and the absorber can be calculated by applying an energy balance around the chiller:

$$\dot{Q}_{cool} = \dot{Q}_{abs} + \dot{Q}_{cond} = \dot{Q}_{evap} + \dot{Q}_{gen} \tag{14}$$

And the coefficient of performance results, because the power demand of the pump is small enough to be neglected, as:

$$COP = \frac{\dot{Q}_{evap}}{\dot{Q}_{gen}} \tag{15}$$

The delivered cooling power and the absorbed heating power can be derived from the technical data sheet of the chiller. The two correction factors CCF and HIF are functions $f(T_{cool_{in}}, T_{heat_{in}})$ of the inlet temperatures and can be determined by interpolation from the machine's characteristics. Therefore, the characteristic diagram is mapped into the model using functions, as shown in the following example for the cooling capacity factor:

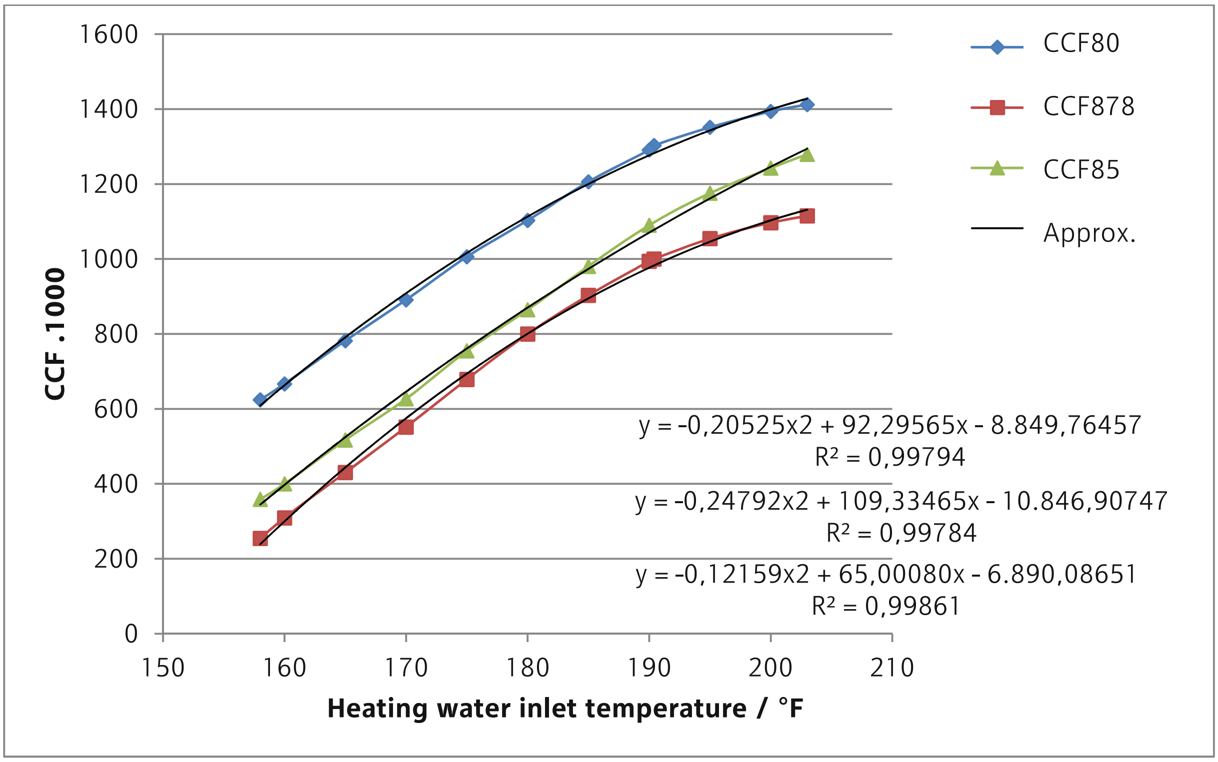

Figure 26: Characteristic diagram for cooling capacity factor of an absorption chiller, ex. for parameterization [125, p. 53]

$$CCF80 = -0{,}20525 \frac{1}{{}^{\circ}\mathrm{F}^2} T_{heat_{in}}{}^2 + 92{,}296 \frac{1}{{}^{\circ}\mathrm{F}} T_{heat_{in}} - 8849{,}8 \tag{16}$$

$$CCF878 = -0{,}24792 \frac{1}{{}^{\circ}\mathrm{F}^2} T_{heat_{in}}{}^2 + 109{,}33 \frac{1}{{}^{\circ}\mathrm{F}} T_{heat_{in}} - 10847 \tag{17}$$

$$CCF85 = -0{,}12159 \frac{1}{{}^{\circ}\mathrm{F}^2} T_{heat_{in}}{}^2 + 65{,}001 \frac{1}{{}^{\circ}\mathrm{F}} T_{heat_{in}} - 6890{,}1 \tag{18}$$

The heat medium flow correction given in the manufacturer's data sheets can be approximated in a similar way. The power of an absorption chiller decreases with reduced heating water mass flows. Therefore, by purposeful reduction of the mass flow a limited part load control until approx. 75% of the nominal power of the machine can be executed. Due to the model design the inlet temperatures of the heating and cooling medium are required. Similar to the solar thermal collector they can be set as parameters or be supplied by the grid model. Furthermore as a control input the required heating power must supplied.

Component Model: Adsorption Chiller

The model, created as part of the bachelor thesis of Stefan Pitschuch [126], is quite similar to the absorption chiller model. It requires the inlet temperatures and mass flows as input variables or parameters. These are used to simulate the outlet fluid temperatures, the produced cooling power, as well as the absorbed heat flow and the thermal efficiency. Although adsorption chillers operate discontinuously the behavior was approximated as continuous in the model.

The emitted refrigerating power $\dot{Q}_{cold}$, the heating demand $\dot{Q}_{heat}$, and the required cooling power $\dot{Q}_{cool}$ result from:

$$\dot{Q}_{heat} = HWE\ HVPF\ \dot{Q}_{heat\_nom} \tag{19}$$

$$\dot{Q}_{cold} = \dot{Q}_{heat}\ COP\ CVPF \tag{20}$$

$$\dot{Q}_{cool} = \dot{Q}_{heat} + \dot{Q}_{cold} \tag{21}$$

In which $\dot{Q}_{heat_{nom}}$ represents the nominal heat demand and can be taken from the data sheets of the machine. The hot water efficiency (HWE) and the COP represent the dependence of the chiller efficiency on the heating water temperature, while the heating volumetric performance factor ($HVPF$) and cooling volumetric performance factor ($CVPF$) depict the dependence on the mass flow of heating water. All values are usually specified in the machine's set of characteristic curves, which are represented in the model by means of polynomial functions, similar to the absorption chiller model. Again the inlet temperatures of the heating and cooling medium are required, since the machine's performance characteristics depend on them, and a control signal communicating the required heating power must be supplied.

Component Models: Heat Pumps and Compression Chiller

Heat pumps and compression chillers can be modeled in the same way, simply inverting the hot and the cold side. Two different modeling approaches are proposed here and shall be described upon the heat pump example.

Usually the performance of a heat pump is mainly determined by desired supply line temperature and the temperature of the cold side medium $T_{cold_{in}}$ on which the heat flow $\dot{Q}_{heat}$

and the electrical power demand P_{el} depend. Assuming that the supply line temperature is kept at a constant level, the COP is only dependent on the cold side medium temperature

$$COP = (a_0 + a_1\, T_{cold_{in}} + a_2\, T_{cold_{in}}{}^2 + a_3\, T_{cold_{in}}{}^3) \tag{22}$$

If the heat demand $\dot{Q}_{heat_{dem}}$ is a known input and can be covered by the heat pump the power demand P_{el} can be calculated as

$$P_{el} = \frac{\dot{Q}_{heat}}{COP} \tag{23}$$

and the heat demand at the cold side of the heat pump is determined by an energy balance:

$$\dot{Q}_{heat} = \dot{Q}_{cold} + P_{el} \tag{24}$$

The second, even more simplified calculation method, calculates the COP solely based on the ratio of the heat demand and nominal heat flow, which is also sometimes listed by the manufacturer. This method is generally suitable for heat pumps with fairly constant temperatures at the hot and cold side, since the COP varies with the temperature difference to gap, where part load performance is of interest

$$COP = (a_0 + a_1\, \frac{\dot{Q}_{heat_{dem}}}{\dot{Q}_{heat_{nom}}} + a_2\, (\frac{\dot{Q}_{heat_{dem}}}{\dot{Q}_{heat_{nom}}})^2 + a_3\, (\frac{\dot{Q}_{heat_{dem}}}{\dot{Q}_{heat_{nom}}})^3) \tag{25}$$

Component Model: Cooling Tower

The inputs of the cooling tower model, which was developed within the bachelor thesis of Philipp Cooberg [127] are dictated by the environment or by the connected chilled water users, which determine the conditions of the ambient air and the incoming water mass flow. In addition, the desired outlet water temperature $T_{w_{out}}$ acts as a control input to the model. The cooling tower is parameterized by means of the cooling tower constant k_0 and the characteristic of the fan efficiency, which is stored in the model as a function. The model calculates the cooling power transferred to the water, the fresh water demand and the fan power. Using the wet bulb temperature of the ambient air T_{k1} the degree of cooling η_A and the air ratio λ is calculated:

$$\eta_A = \frac{\left(T_{w_{in}} - T_{w_{out}}\right)}{\left(T_{w_{out}} - T_{k1}\right)} \tag{26}$$

$$\eta_A = k_0\, \left(1 - e^{-\lambda}\right) \tag{27}$$

The air ratio λ represents a ratio of the actual amount of air to the minimum amount of air. The latter is a characteristic value of the cooling tower. Thus the required air mass flow is obtained. With the help of the energy balance, the enthalpy of moist air at the inlet and outlet and the steam mass balance all the missing state variables of the incoming and outgoing flows can be calculated.

$$\dot{m}_{w_{in}}\, c_{p_w}\, T_{w_{in}} + \dot{m}_{air_{in}}\, h_{air_{in}} + \dot{m}_{FW_{in}}\, c_{p_w}\, T_{w_{out}} = \dot{m}_{w_{out}}\, c_{p_w}\, T_{w_{out}} + \dot{m}_{air_{out}}\, h_{air_{out}} \tag{28}$$

$$h_{air_{in}} = c_{p_{air}}\, T_{air_{in}} + c_{p_{vap}}\, T_{air_{in}}\, X_{in} + r_0\, X_{in} \tag{29}$$

$$h_{air_{out}} = c_{p_{air}}\,T_{air_{out}} + c_{p_{vap}}\,T_{air_{out}}\,X_{out} + r_0\,X_{out} \tag{30}$$

$$X_{out} = X_{in} + \frac{\left(h_{air_{out}} - h_{air_{in}}\right)}{Le\,\dfrac{\left(h_{sw} - h_{air_{in}}\right)}{\left(X_s - h_{air_{out}}\right)} + \left(h_{gw} - h_{g0}\,Le\right)} \tag{31}$$

Le is the Lewis Number. X_s is the water load of saturated air. Further sate variables are the enthalpy of saturated humid air at water inlet temperature h_{sw}, the enthalpy of saturated steam at water inlet temperature and at 0°C, h_{gw} and h_{g0}. Since, this model was implemented in Modelica, the values can be obtained from the Modelica library, which provides the relations to calculate the state variables. Otherwise, these need to be implemented in the model as well.

From the state variables and mass flows the heat flow and the demand of fresh water can be calculated. The ventilator operating power is derived from the ventilator characteristics, which is described as a function in the model.

Component Models: Boiler and CHP

The models for boilers and CHP rely on the characteristics of the CHP data sheet that are approximated by polynomial functions, similar to the chiller models described above. They are, however, significantly simpler since it is in general not necessary to interpolate between characteristics, because the operational state of the CHP is influenced significantly only by one variable, the load. Return line temperatures generally have only minor effect on the performance and the effect can be ignored when modeling. Therefore, only one characteristic, not a set, had to be modeled. In order to fully describe a CHP unit three characteristics are necessary; one for the electricity and the heat production and one for the fuel consumption E_{in}:

$$P_{el} = P_{el_{nom}}\,(a_0 + a_1\,LF + a_2\,LF^2 + a_3\,LF^3) \tag{32}$$

$$\dot{Q}_{heat} = \dot{Q}_{heat_{nom}}\,(b_0 + b_1\,LF + b_2\,LF^2 + b_3\,LF^3) \tag{33}$$

$$E_{in} = E_{in_{nom}}\,(c_0 + c_1\,LF + c_2\,LF^2 + c_3\,LF^3) \tag{34}$$

LF stands for load factor and is derived from the demanded heat or electricity, depending whether the CHP is heat driven or electricity driven, divided by the respective nominal power. In case of a heating device without electricity generation, equation (42) is obsolete. By applying an energy balance around the unit, the dissipated waste heat can be calculated:

$$E_{in} = P_{el} + \dot{Q}_{heat} + \dot{Q}_{wh} \tag{35}$$

In case the thermal mass of the CHP or boiler has a significant influence in terms of temporal delay of the heat release the energy balance can be extended by a dynamic term and a temperature dependent expression for the heat loss. However, this modeling approach requires the knowledge of some physical properties of the CHP or boiler.

$$E_{in} = P_{el} + \dot{Q}_{heat} + k_{CHP}\;A_{CHP}\,(T_{amb} - T_{CHP}) + C_{p_{CHP}}\,dT_{CHP} \tag{36}$$

Due to the generic description using solely characteristic based relation the models can be used to model any kind of CHP operated with solid, liquid or gaseous fuel.

4.4.2. Secondary Systems

Secondary energy systems consist of all systems used to distribute and store energy within the energy system. As mentioned in Chapter 4.1 distribution systems, the connecting networks in particular, are usually modeled in a deductive modeling process, because their configuration is mostly well known and they are usually quite unique in realization. But still some components can be supplied by a library, namely storage devices and distribution systems. In this library electrical storage devices (batteries), several types of thermal storages (simplified, stratified, activated core and latent), as well as pumps and ventilators were integrated.

Component Model: Electrical Storage

The model was created for the not yet completed bachelor thesis of Sara Schiek in order to describe different types of electrical storages. The output power of the battery depending on the type of battery, on the discharge current, the rated voltage and the storage capacity is simulated. The different battery types have different discharging behavior, which is derived from characteristics. These discharge curves represent the voltage depending on the capacity and can be approximated as a polynomial function. Figure 27 shows the discharge curves of some established battery types at a certain discharge rate.

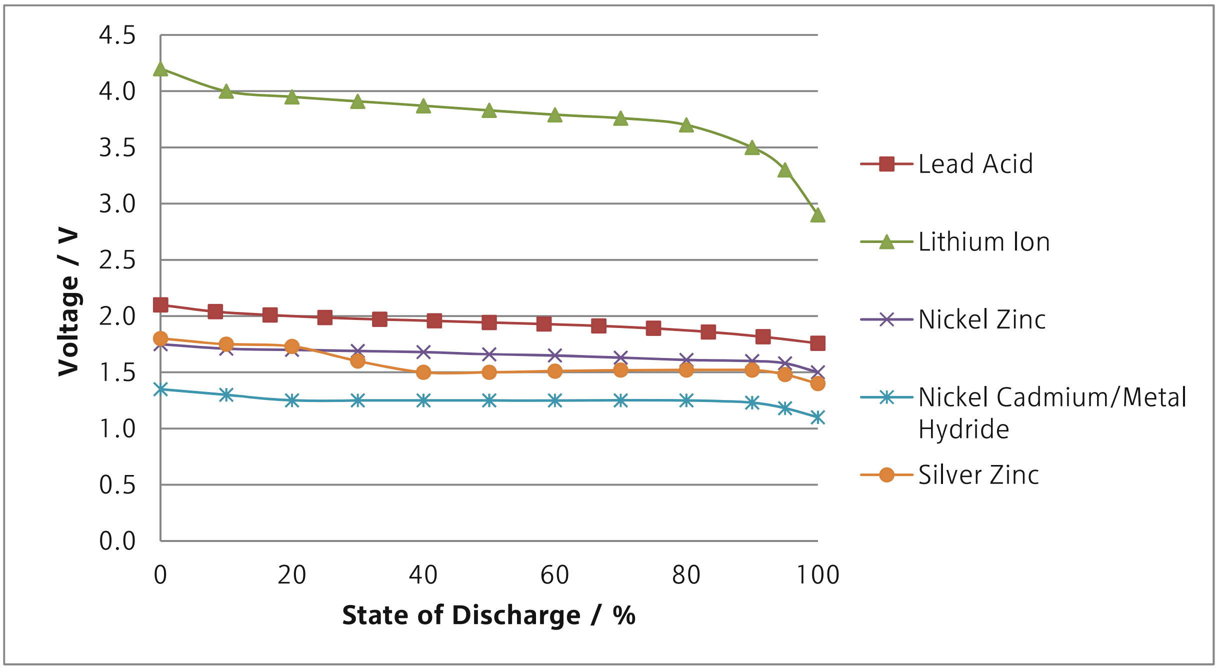

Figure 27: Discharge curves of different battery types, C/5-rate [128]

The dependence of the discharge curve from the discharge current (higher discharge current results in lower actual capacity) is adjusted by the Peukert equation

$$t\,I = C_{p_{bat}} \left(\frac{C_{p_{bat}}}{I\,H}\right)^{k-1} \tag{37}$$

in which t is the time in hours until discharge, $C_{p_{bat}}$ the Peukert capacity, I the discharge current in Ampere, H the nominal charging time in hours and k the Peukert exponent. With the voltage U as well as the discharge current I known, the power of the battery can be calculated

$$P = U\, I \tag{38}$$

Thus, the performance of the battery is determined as a function of the charge state.

Component Models: Heat Storage and Stratified Heat Storage

The heat storage model was realized by an energy balance around the storage volume. The incoming and outgoing heat flows as well as the losses through the storage wall were taken into account.

$$m_{storage}\, c_{p_{storage}}\, dT_{storage} = \dot{Q}_{loss} + \dot{Q}_{in} - \dot{Q}_{out} \tag{39}$$

$$\dot{Q}_{loss} = -k_{wall}\, A_{wall}\, (T_{storage} - T_{amb}) \tag{40}$$

This heat storage model is of course applicable for solid and fluid storage solutions. By the discretization of the reservoir volume into a series of vertically stacked volume elements the model was developed into a simplified stratified storage tank model for fluid storage solutions.

For each stratified volume segment an energy balance was formulated. Figure 28 shows the energy flows entering and exiting the volume element.

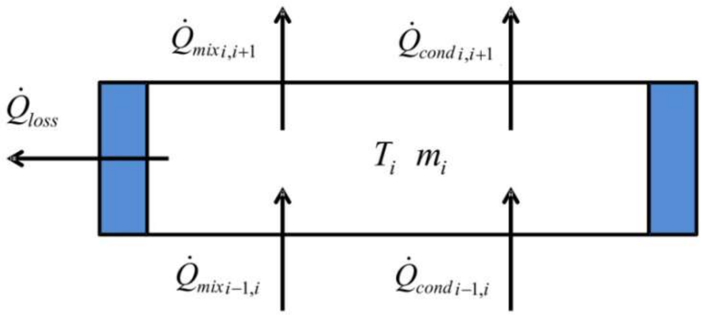

Figure 28: Volume segment of stratified storage with heat flows

The energy balance for the volume element therefore results as:

$$dT_i = \frac{(-\dot{Q}_{loss} - \dot{Q}_{mix_{i-1,i}} - \dot{Q}_{cond_{i-1,i}} + \dot{Q}_{mix_{i,i+1}} + \dot{Q}_{cond_{i,i+1}})}{m_i\, c_{p_{fl}}} \tag{41}$$

with the heat flows:

$$\dot{Q}_{loss} = k_{wall}\, A_{wall}\, (T_i - T_{amb}) \tag{42}$$

$$\dot{Q}_{cond_{i-1,i}} = A_{seg}\, k_{seg}\, (T_i - T_{i-1}) \tag{43}$$

$$\dot{Q}_{mix_{i-1,i}} = \frac{m_i\, c_{p_{fl}}}{\tau}\, (T_{i-1} - T_i) \tag{44}$$

In which A_{wall} and k_{wall} are the outer surface of the volume and the heat transfer coefficient through the storage wall. And A_{seg} and k_{seg} the surface of the volume element to the adjacent element and the corresponding heat transfer coefficient between the fluid segments. τ represents the time constant for mixing of the fluid between the two segments, which represents the convective fluid movements within the tank.

Component Model: Latent Heat Storage

For the model, created as part of a bachelor thesis of Danijel Djordjevic [129], a finite volume method was selected and the storage was discretized as shown in Figure 29.

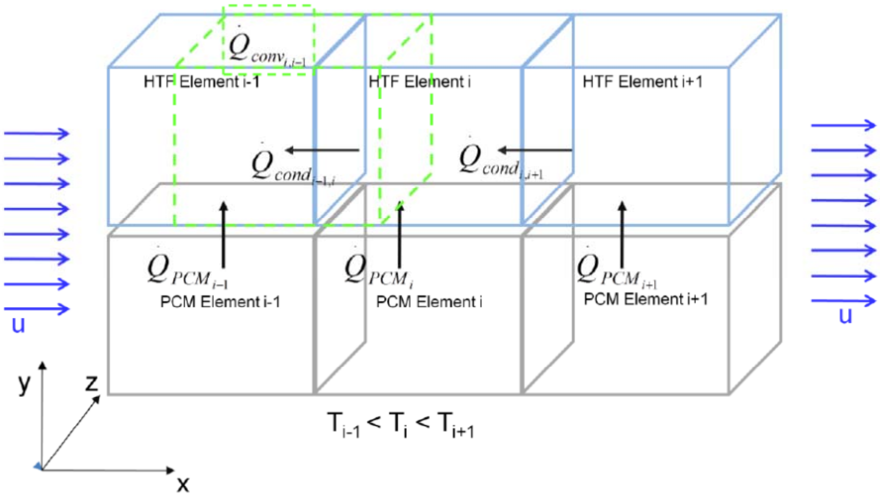

Figure 29: Discretization of the latent heat storage [129, p. 23]

The three relevant heat transport processes in the storage are described as follows. Conductive heat transport due to spatial differences in temperature (Fourier's Law):

$$\dot{Q}_{condu} = f\; k_{HTF}\; \frac{\partial {T_{HTF}}^2}{\partial x^2} \tag{45}$$

Energy transfer by means of convection:

$$\dot{Q}_{conv} = f\; \rho_{HTF}\; c_{p_{HTF}}\; u\; \frac{\partial T_{HTF}}{\partial x} \tag{46}$$

Conductive heat transfer from the PCM element to the heat transfer fluid (HTF) element:

$$\dot{Q}_{PCM} = \alpha\; A\; (T_{HTF} - T_{PCM}) \tag{47}$$

The energy balance around a volume element of the heat transfer fluid is therefore obtained as:

$$\dot{Q}_{HTF} = \dot{Q}_{PCM} + \dot{Q}_{condu} - \dot{Q}_{conv} = f\; \rho_{HTF}\; c_{p_{HTF}}\; \frac{\partial T_{HTF}}{\partial t} \tag{48}$$

In which the indices HTF denotes the fluid, PCM the storage material, u the flow velocity of the fluid and the parameter f the volume fraction of the heat transfer fluid of the total volume.

Component Model: Concrete Core

The concrete core model is a modification of the general storage model. It approximates the concrete core as a storage capacity without local temperature differences, and consists of a simple energy balance as well. But since concrete cores are in most cases designed to dissipate heat or cold to their surrounding, no losses and outgoing heat flows are taken into consideration, only the heat flows in the zones above and below, as well as the heat flow injected via core activation $\dot{Q}_{in}$. This results in the following energy balance:

$$dT_{TABS} = \frac{(\dot{Q}_{in} - k_u\, A_u\, (T_{TABS} - T_u) - k_d\, A_d\, (T_{TABS} - T_d))}{c_{p_{TABS}}\, m_{TABS}} \tag{49}$$

Where the indices u and d represent the directions to the zones above and below (up/down) and $TABS$ the concrete core (thermally activated building system).

Model: Thermal Zones Building

In addition to the electrical and thermal heat storage devices a model for thermal zones of a building was included into the library as it is an important thermal influence and represents an additional storage potential. Furthermore it interfaces with the concrete core. The thermal zone of the building was modeled as a substitutional heat storage capacity with thermal resistances which influence the incoming and outgoing energy flows. Several heat flows influence the thermal balance in the thermal zone significantly and were included in the model. The internal loads $\dot{Q}_{gain_{int}}$, the heat flows injected by the concrete cores above and below ($\dot{Q}_{TABS_u}$, $\dot{Q}_{TABS_d}$), the transmission losses to the environment and to adjacent thermal zones:

$$\dot{Q}_{loss_{tr}} = U_{out}\, (T_{zone} - T_{amb}) \tag{50}$$

$$\dot{Q}_{int_{tr}} = U_{zone,j}\, (T_{zone} - T_j) \tag{51}$$

with U_{out} and $U_{zone,j}$ as the heat transfer coefficients to the external and the adjacent zones. Furthermore, the infiltration losses, due to leakage were considered:

$$\dot{Q}_{loss_{inf}} = \frac{n}{3600\,\frac{\mathrm{s}}{\mathrm{h}}}\, V_{zone}\, \rho_{air}\, c_{p_{air}} (T_{zone} - T_{amb}) \tag{52}$$

where n is the air change rate in $1/\mathrm{h}$. The gains by solar radiation on windows are also included in the model and are calculated by means of the transmittance g and the incident solar radiation I:

$$\dot{Q}_{gain_{solar}} = g\, A_{window}\, I \tag{53}$$

For the solar radiation either only the diffuse radiation, or the direct and diffuse radiation are taken into account, depending whether the shading is activated. Figure 30 shows an overview of the thermal zone.

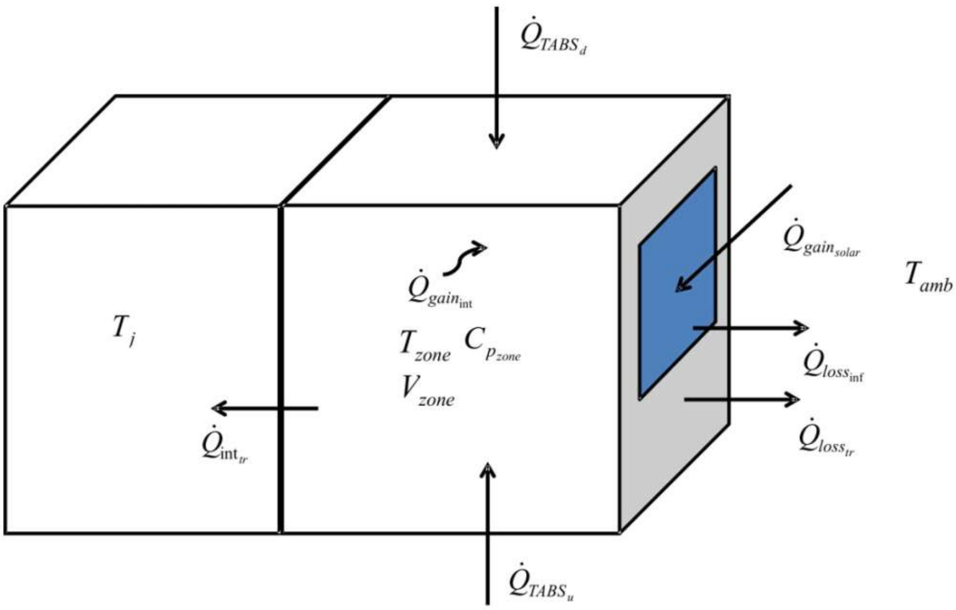

Figure 30: Overview of the heat flows in the thermal zone

Ultimately, the energy balance can be formulated:

$$dT_{zone} = \frac{(\dot{Q}_{gain_{int}} + \dot{Q}_{TABS_u} + \dot{Q}_{TABS_d} + \dot{Q}_{gain_{solar}} - \dot{Q}_{loss_{tr}} - \dot{Q}_{int_{tr}} - \dot{Q}_{loss_{inf}})}{C_{p_{Zone}}} \tag{54}$$

Component Models: Pumps and Ventilators

The models of pumps, fans, heat exchangers are modeled by simple characteristics. Based on the operating point, which is determined by the mass flow to be transported, the power demand is calculated:

$$P_{el} = P_{nom}(a_0 + a_1 \frac{\dot{m}}{\dot{m}_{nom}} + a_2 (\frac{\dot{m}}{\dot{m}_{nom}})^2) \tag{55}$$

Models of Networks and Control

The models of the networks are realized by energy and sometimes mass balances. Due to the fact that the system configuration and the related controls are usually individual solutions in realization no generally applicable models can be provided in a library. Unique solutions must be found by the modeler. Modeling examples for the grids in connection with the components provided in the library and consistent with the respective model requirements can be found in Chapters 5 and 6, realized for the presented application cases.

5. Application to Design of Energy Efficient Production Facilities

5.1. General Project Description an Initialization Phase

As described in the introduction, the energy demand of the production industry accounts for a major part of society's total energy consumption, thus offering a large leverage for energy efficiency measures. The research project INFO was assigned to the task of developing a holistic planning instrument for optimizing the energy efficiency of production facilities and halls. When the project started in 2010 sensitivity towards energy efficiency had just started to develop within the industry. Before the critical success factors of the industrial manufacturing sector had been the increase of productivity and decrease of costs. A German study carried out in 2009 showed that even fairly basic energy efficiency measures, such as the use of speed controlled drives, were not even used by half of the surveyed companies [130]. But due to additional demands, such as legislative pressure, consumer awareness and rising energy costs, energy efficiency became an increasingly important topic in the manufacturing industry by then. Therefore, numerous research initiatives started to engage themselves with the topic.

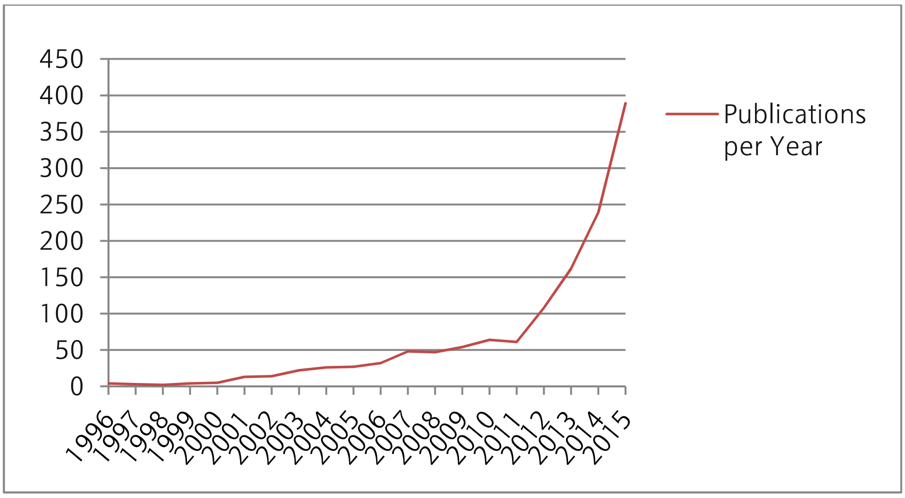

Figure 31: Development of publications concerning "energy efficiency" in the "Journal of Cleaner Production"

Some of the research initiatives had started to identify the demand and the potential. [13] quantified the achievable savings by reviewing numerous case studies between 30% and 65% depending on the industry sector.

In order to reduce a producing company's energy consumption many studies focused on improving the efficiency of the production processes. Significant potentials could be exploited with this approach, such as [131] and [132]. Another important sphere of activity identified by [133, p. 348] is the efficient operation of the infrastructural facilities of production plants. This suggests that combining the mentioned approaches could show even better results, which has also been demonstrated successfully for instance in [134] and [135].

However, research ([136]–[140]) has shown that efforts in this direction are often inhibited by the lack of information, financial and human resources, unpredictable financial risk, long return on investment times and negative impacts on the production process. In order to overcome this so called "energy efficiency gap", [137] and [133, p. 350] suggest that comprehensive methods for energy monitoring and management as well as reliable tools for the assessment of optimization potentials and their financial impact are needed.

Therefore, a considerable amount of research has been devoted to develop energy efficiency assessment methodologies, monitoring and management tools. But not only tools and methodologies to assess the plant operation with regards to energy efficiency are needed. The right design of newly built plants or well elaborated retrofits play an important role too. Kovacic et al. states that careful assessment of a future building's behavior plays a crucial role for the determination of the development of resource and energy consumption, as well as costs during the building life cycle [141]. As shown in Figure 32 in the first stages of the planning process the potential for changes and therefore for optimization is still very large at a low cost. In the later phases it decreases rapidly and comes at a much higher cost. It can also be seen in the figure that integrated planning can significantly reduce the life cycle cost of buildings.

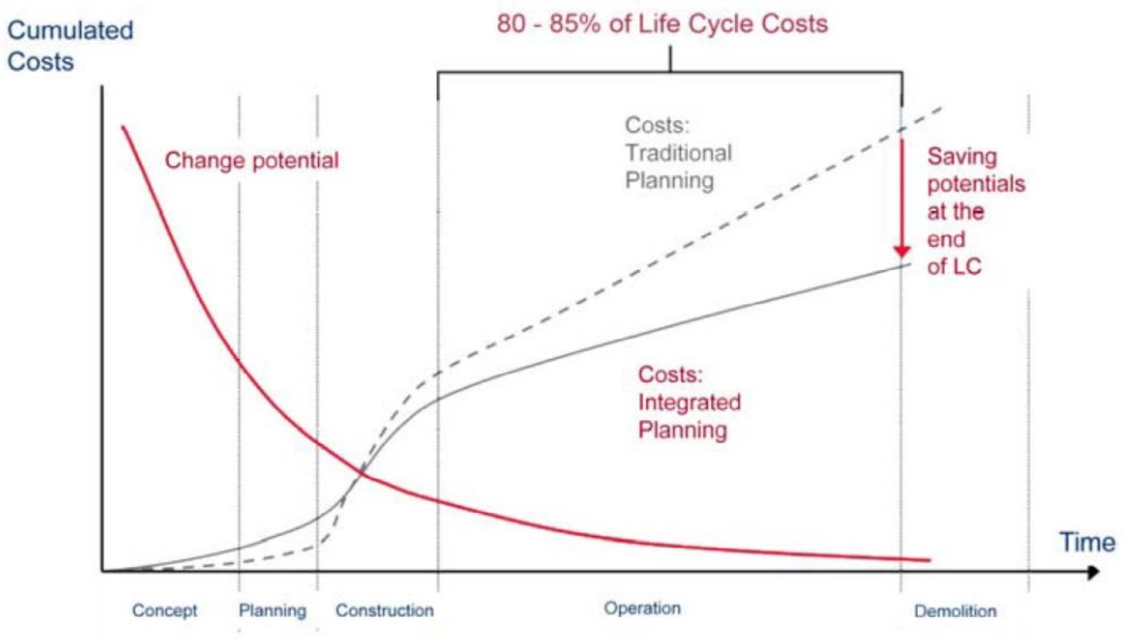

Figure 32: Cost development vs. change potential over the building life cycle [141]

In this context the project INFO focused on the development of a simulation based planning support for production facilities. It integrated several optimization fields within the facility and demonstrates their influence on each other. It was meant to be a decision support instrument, which enables planners to assess the performance of the building and the production in an early planning phase.

This project goal was reflected in the project structure and the project team. Figure 33 gives an overview of the tasks within the project. Further goals of the project, apart from developing the simulation framework, were also to demonstrate its usability with a case study, to publish a roadmap for energy efficient production and to use the simulation results as reference values for an energy performance certification for industrial buildings. Prior to starting with the design and implementation of the simulation framework, a work package was dedicated to analyzing the business processes of manufacturing companies and defining the targets of the simulation. Based on these findings the models for the main optimization fields (production, building, energy system) were to be developed and later on integrated into a simulation framework. The modeling process was to be supported by data collection from real production sites. As a proof of concept a case study with the newly developed tool was to be performed.

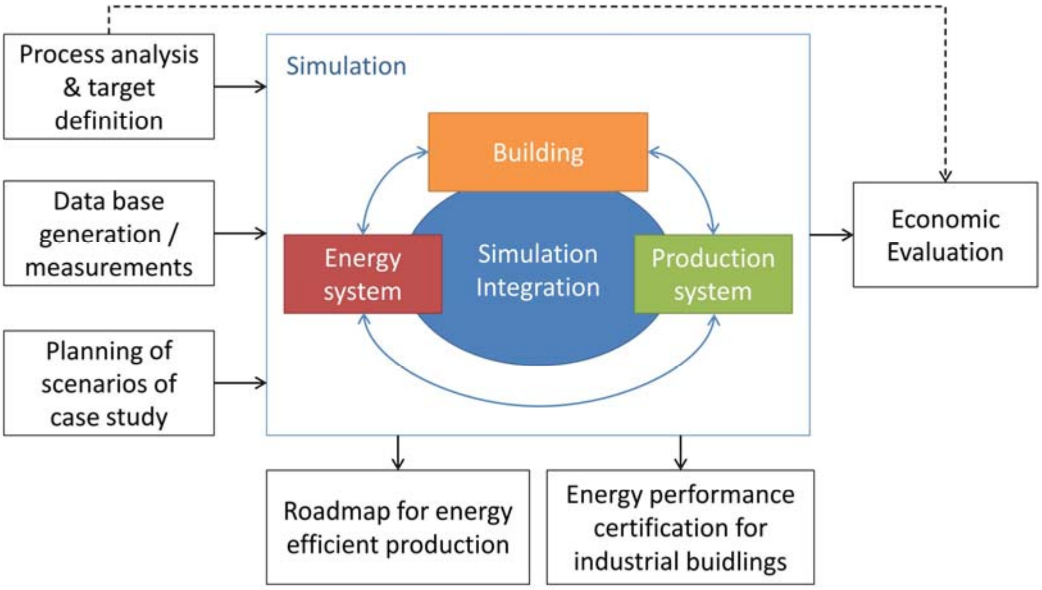

Figure 33: Structure of tasks of the INFO project

The consortium included a number of manufacturing companies, an interdisciplinary team of researchers from the disciplines of architecture, informatics, economies, mathematics, civil- and mechanical engineering. Concerning a detailed role definition the following expectations and expertises could be defined:

- Stakeholders; three basic groups of stakeholders could be defined:
    - Funding agency (simulation sponsor) (1) had an interest in obtaining a valid, applicable tool with reuse value.
    - Manufacturing companies in the consortium (2): Since a case study had to be delivered at the end of the project, one of the participating companies obtained the benefits of the simulation results, which were to be meaningful and credible. In return the manufacturing companies had to provide certain data and information for the simulation.
    - Simulation result users (3): Apart from the case study the simulation results also served as a base for further project outcomes (energy performance certification and roadmap). Therefore, the researchers tasked with the development of these project outcomes had certain expectations concerning the significance and validity of the results. In the case of this project this group also possessed expert knowledge in building sciences.
- Domain Experts; a number of domain experts were represented in the simulation team, most of which possessed a certain proficiency in modeling and simulation as well:
    - Manufacturing companies in the consortium (2): As well as being benefactors of the simulation, the involved companies were also the main source of expert knowledge on the specifics of their manufacturing systems and the needs and limitations when facing the optimization of real-world productions.
    - Simulation result users (3) were also domain experts in building sciences (see above).
    - Architects and building planners (4): When planning new facilities, the planner's expertise in how to assemble working systems is crucial and also supplies the majority of input parameters for the simulation.

- Industrial building experts (5) were experienced researchers in terms of all aspects of integral and sustainable planning of manufacturing facilities as well as building information modeling (BIM).
- Production research experts (6) participating in the project possessed extensive knowledge of production systems on process, component and system level and the according measurement and data collection methods as well as some knowledge about modeling of the systems.
- Energy system experts (7) contributed expertise considering the design of the building service systems and their simulation.
- Economic experts (8) contributed knowledge about analysis of business processes and target definition, as well as the processing of the energy related simulation results into meaningful KPIs.

- Simulation experts: Apart from several domain expert groups being experts in their domain specific modeling and simulation methodologies (industrial building experts, production research experts, energy system experts), two specific simulation expert groups participated in the project:
  - Modeling and Simulation experts (9) added expertise in all fields of M&S concepts and approaches on an abstract non-domain related level.
  - Building science experts (10) contributed their vast expertise in thermal building simulation.

Altogether, the roles in the project can be mapped as shown in Figure 34. As it can be seen this project is a classic example in which the roles of stakeholders and domain experts as well as domain experts and simulation experts coincide. Concerning familiarity with tools the industrial building experts favored BIM tools such as Revit, production research experts were familiar with Matlab, energy system experts worked with Modelica/Dymola and TRNSYS and building science experts preferred EnergyPlus or TRNSYS.

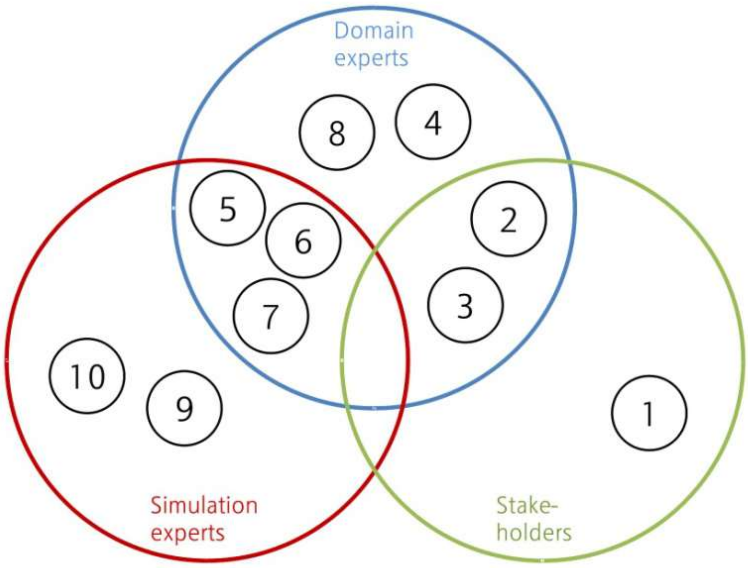

Figure 34: Role definition INFO project

5.2. Problem Formulation and Requirement Definition

After defining the roles within the project team in context with the simulation and assessing the competences, the process of problem formulation and requirement definition was started in the project team. Partly the objectives and the system were already defined in the proposal of the research project which stated that the simulations would enable industrial companies to systematically analyze and optimize the eco-efficiency of their production processes and equipment. Production sites in Austria were regarded as the primary application fields.

This relatively unspecific goal definition led to a rather lengthy and tedious discussion process to determine the real objectives and specifications of the simulation undertaking. Since the project team was also quite inexperienced in carrying out interdisciplinary research projects and unfamiliar with concepts and approach of other domains a number of misunderstandings and disagreements occurred in the course of this process. For instance, for several disciplines the term simulation implied the replication of a process over time (transient simulation), while planners and architects in the team had more of a static, virtual model of a building, such as comprised using BIM techniques, in mind. It took some time to discover this terminological disagreement and resolve the matter. Therefore, as mentioned in the reference model description, it is advised to compile a glossary, which wasn't done in this particular project.

System description

Agreeing on the system description was the easier part of the discussion process. It was quite clear from the proposal formulation that the system under study for the M&S study was a production company and that economic as well as ecological influences had to be taken into consideration. For system analysis 5 optimization fields were identified, that should be analyzed, modeled and ultimately integrated into the simulation (see Figure 3) focusing on the energy flows.

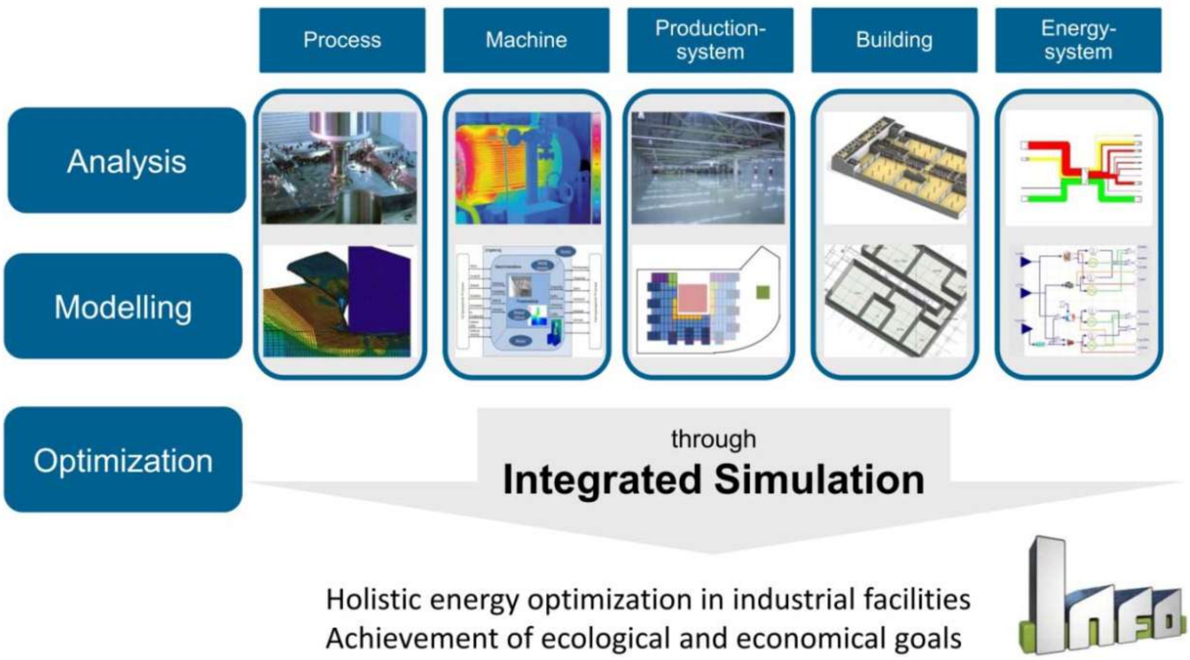

Figure 35: Optimization fields in a production plant as identified in project INFO

It was also clear that the simulation followed a "to-the-gate" approach i.e. that only factors that happened inside the respective productions site were taken into consideration. This limits the energetic observations to final energy only and excludes external transport as an optimization field.

Data and information collection

Parallel with the discussion process the collection of data and information started. The data collection branched in several directions. Analysis of the identified optimization fields was carried out to uncover optimization potentials and also to find suitable modeling approaches for the respective field. Also the collection of data, for model parameterization was partly started in this phase. That was probably a little bit premature, since the idea of the actual model related data requirements was only starting to form in this phase of the project. And most importantly in a series of interviews with the manufacturing companies their preconditions, needs and limitations were identified.

This process quickly showed that for the majority of companies the motivation to invest into energy saving measures was competitiveness driven. It also made clear that the boundaries for applying optimization strategies were tightly set. Naturally, the fear of affecting product quality in a negative way turned out to play an important role. Loosing flexibility to adapt the production to changing product portfolios was also considered a criterion for exclusion and last but not least accepted return on investment (ROI) times were quite short.

Objective specification

The objectives what the actual results of the simulation could be, was still very unclear and clouded during the discussion and information collection process. After about one year (sic!) of discussion a more concise idea of the objectives started to form. A target specification document, dated at almost a year and a month after the project started, states:

> *The simulation enables the comparison of scenarios of system configuration concerning the optimization criteria: economic criteria (operational result) and ecological criteria (climate relevant emissions) based on concrete planning of an object. For that purpose a life-cycle cost oriented cost benefit analysis is used. The objective is to compare the expected profits before tax of the individual scenarios under consideration of building, production plants and energy in order to be able to make a qualified investment decision. Furthermore, objectives of the simulation are to depict the trajectories of energy flows (e.g. heat flows, electricity) and other relevant variables of the system, as well as to identify the key parameters of the energetic behavior of manufacturing companies.*[142]

Based on the findings of the problem formulation the intended uses, use case and requirements were specified.

Intended uses

The intended uses of the simulation tool could easily be derived from the problem formulation, since most of them were already implied within. The fact that the information collection showed such tight boundaries, led to the conclusion that infrastructural energy efficiency measures can only be implemented feasibly in plants that are newly build or undergo a major retrofit. Therefore, it was decided to limit the application field to planning of such, and the intended uses of model and simulation could be formulated as:

- The simulation is intended to be used as a supporting tool in the planning process of newly built production plants or major retrofits.
- It is designed to compare scenarios of different system configurations of the production plant based upon concrete planning of the scenarios.
- The simulation is intended to be used to identify and analyze energy flows and their dependence on key parameters in manufacturing companies.
- The conceptual model is intended to be used as a communication tool between experts when analyzing system correlations and influences.

In addition to the intended uses it was also clearly defined what the model and simulation are not intended for. Since the focal points of the model are the energy flows within the production plant, it is not intended to be used for any other optimization task apart from increasing energy efficiency and implementing renewables. Furthermore, it is not intended to serve as the basis for a design simulation with an integrated optimization algorithm to find the ideal set of parameters. It is rather designed to be the foundation for simulation of varying pre-selected scenarios to be manually compared with each other in terms of specified output key data.

Use cases

The typical use case for the model and simulation is in an integrated planning process, where a new facility is planned and built. Based upon the core requirements of the client, which usually includes as a minimum the location, type of production to be housed, and other types of use, a team of architects and planners will come up with recommended scenarios for the building and its content.

These scenarios including structural information and the data to parameterize the simulation are given to the simulation team. Each expert for a specific area (building, production...) realizes a model, with a minimum of effort involved, because the reuse of existing models and domain specific simulation environments is possible. Due to predefined interfaces the submodels can easily be integrated into the framework and executed fairly swift. The modeler obtains energy demand and emission data, as well as economic KPIs. Considering the economic analysis, in this case the functional unit of the life cycle analysis is not the product, but has to be the life cycle of the plant. Furthermore, rather than analyzing the whole economic performance of the company, which would not be within the scope of the study, only the influence of the energy use is taken into consideration i.e. a differential analysis is performed.

The results are reported back to the planning team and the client in order to provide decision support upon the ecologic impact of the scenarios and the economic implications.

Requirements

Based on the intended uses and the use cases the functional and non-functional requirements were defined as follows:

Functional:

- The conceptual model is designed as a universally applicable model of a production facility and therefore, documents all potentially existent and relevant parts of a production facility.
- The entire facility can be simulated with the model. Therefore, all energy consuming, supplying and converting system parts are represented in the model.

- The model is focused on energy flows and all relevant energy flows are depicted in the model.
- Influences and relations of energy using, supplying and converting system parts are represented in the model.
- All energy relevant control strategies are represented in the model.
- Representations of planning activities are integrated into model and information flows from planning to the simulation are documented.
- Total energy demand and emissions produced are calculated by the simulation.
- An economic analysis is implemented in the model and simulation or conducted based on the simulation output data.
- Environmental influences (climate, economic developments) are considered in model and simulation.
- The conceptual model is formulated in a generic way that ensures applicability to all types of production plants.
- The simulation is of transient nature and is performed over a simulation time of at least a year.

Non-functional:

- The conceptual model is represented and documented in a way it can serve as a communication tool for experts.
- The conceptual model enables the involvement of multiple simulation tools.
- Existing models of system parts can be reintegrated into the model.
- The conceptual model enables the reuse of domain specific simulation tools but is independent of any simulation tools that eventually would be used to carry out the simulation.
- The execution time of the simulation stays within limits (coffee-break, lunch-break).

It should be noted at this point that the described process was by no means linear and that several of the specifications described above were discovered during the conceptual modeling process and had to be added afterwards. This effect is also certainly due to the fact that the conceptual model provided the much needed communication tool that significantly helped streamline the expert discussion.

5.3. Conceptual Model and Design Model

The next step on the path to the simulation was to develop an underlying conceptual model. As mentioned in the previous section, the aim of the project was the development of a simulation based planning support for production facilities, specifically aimed at energy optimized design. In order to keep the results as flexible in application as possible, the aim of the conceptual model was to design a universally applicable model of a production facility, focused on energy flows. The conceptual model should provide a basis for simulations of the entire facility, enable the involvement of multiple simulation tools, but remain independent of any specific simulation tools.

Therefore, not all the aspects pictured in the model have to be represented in the simulation as well; their selection can be adapted to individual needs. The model also clearly, yet concisely documents all relevant aspects within the whole system and thus serves as a communication instrument for experts of different disciplines collaborating to implement the integrated simulation.

In order to meet the mentioned requirements from the system and the implementation point of view the top-down and bottom-up perspectives and the model structure, based on a generic notion of components, parameters and variables, explained in Chapter 3.3, were applied to the conceptual modeling process.

As defined in the use case, the chosen set of parameters are selected in a planning process, which selects the scenario and ensures parameter consistency. This results in dependencies between parameters of different components and the plan. These dependencies are represented as parameter references to plan elements. The plan elements themselves are not part of the dynamic simulation, but define the parameterization and form a coherent point of reference in order to ensure consistency between the parameters.

Components and Elements of the Model

As demanded by the requirements the conceptual model should be designed as a universally applicable model of a production facility and therefore, document all potentially existent and relevant parts of a production facility. 16 components, which can be presumed to exist in every production facility in one way or another, have been identified. To express that components not only describe physical parts of the system but also abstract parts, two types of components were introduced in accordance with the reference model:

- Physical components (PC) (e.g., building structure, machinery, humans, environment) and
- Information components (IC) (e.g., strategies, algorithms, behavioral patterns, political environment).

A graphical overview of all components as well as the plan elements is shown in Figure 36. Physical components are represented by blue ovals, information components are pictured as ovals with red outlines. Subsequently a short overview of the components of the model will be given.

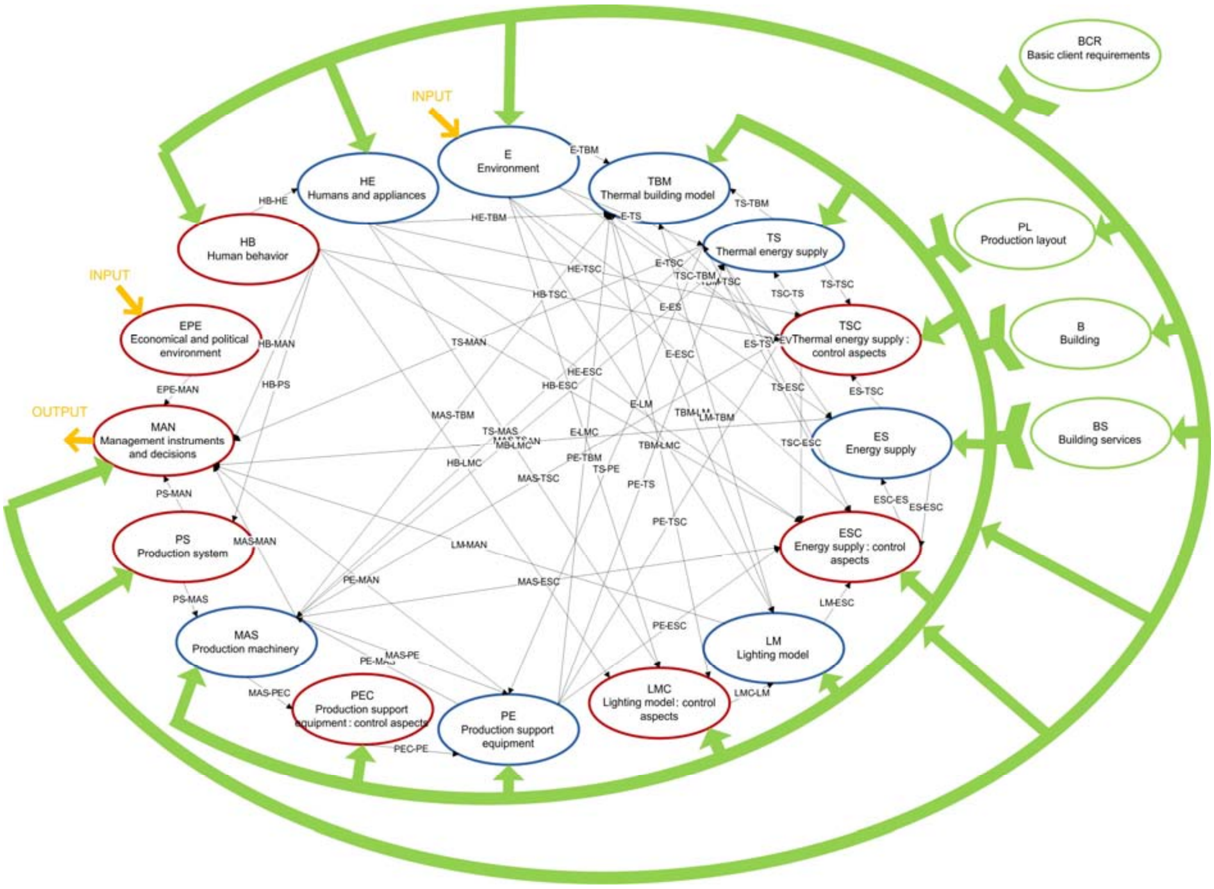

Figure 36: Conceptual model for a production facility ("Spider's Web")

Environment (PC)

This component depicts environmental influences, especially weather conditions at the geographic position of the factory over a year. This is an input component, which means it cannot be influenced by the system and therefore has no input variables.

Thermal building model (PC)

The "Thermal building model" describes the thermal situation in the building. The component contains the relevant parts of the building structure sectioned into thermal zones, but no building services.

Thermal energy supply (PC)

The component "Thermal energy supply" contains all equipment used to supply thermal energy (production, storage, distribution). This encompasses heating, cooling and ventilation of the building's zones, the supply with service water and if necessary process heat as well as cooling of machines and large computer systems.

Thermal energy supply: control aspects (IC)

This component describes the control strategies that are applied to all the equipment related to the thermal energy supply, no matter if they are implemented by automation systems or manually.

Energy supply (PC)

"Energy supply" depicts the supply of all kinds of machines or equipment with all kinds of energy that is not thermal. This includes external supply, internal production, storage and distribution.

Energy supply: control aspects (IC)

The strategies represented by this component coordinate the cooperation of the equipment contained in the component "Energy supply" in order to cover the demand of non-thermal energy of all other components.

Lighting model (PC)

The component contains all relevant parts of the building structure as well as those parts of the building services that affect the lighting situation inside the building. Apart from artificial lighting, this also includes shading and daylight redirecting devices.

Lighting model: control aspects (IC)

This component describes the strategies applied to provide illumination and glare coverage by using the devices contained in the "Lighting model" component.

Production support equipment (PC)

This component contains all the equipment which is needed to support the production machinery and the production process, but has no value-adding function itself. This includes for instance auxiliary supply systems (pressurized air, lubricants) or logistic devices.

Production support equipment: control aspects (IC)

This component describes operation strategies for the component production support equipment.

Production machinery (PC)

"Production machinery" are all machines, machine tools and equipment which directly contribute to the value-adding production process.

Production system (IC)

The production system describes the production planning and scheduling as well as the processes. The information contained in this component allows estimating the utilization of machines and equipment for any certain period of time.

Management instruments and decisions (IC)

This component connects the technical and financial key data provided by the other components in order to assess the system layout in respect of economical criteria (operating results) and ecological criteria (climate relevant emissions). It is an output component, which processes the simulation results and delivers them in the form of KPIs which are significant to a decision maker. The component has no output variables back into the system and thus cannot influence the behavior of the simulated system.

Economical and political environment (IC)

Here, the determining factors of the economical and political environment are described which are essential for the "Management instruments and decisions" component to process the simulation results. This is an input component that cannot be influenced by the system.

Human behavior (IC)

Human behavior depicts when people are present, how many and where they are in the building, what they do and which appliances (not production machinery) they operate.

Humans and appliances (PC)

This part of the system describes the direct, measurable influence by the presence and activity of humans in the building and the appliances they operate in their sole discretion (e.g., computer, coffee maker).

In addition to the 16 components that comprise the dynamic simulation, the model contains four plan elements supplying the components with coherent parameter values. In Figure 36, they are represented by green ovals. First, there are the basic requirements of the client such as the general purpose of the facility or its geographic position. Based on these requirements, the plan elements "Building structure", "Building services" and "Production layout" deliver more detailed parameter specification. This overall "plan" is split into "elements" considering the complexity of the planning process and the fact that these planning tasks are usually carried out by different experts.

Parameters and Variables of the Model

As well as with components, the nature of parameters varies. They can consist of a single physical quantity or can be of a complex composition, such as a control strategy. Again different kinds of parameters are distinguished:

- Physical parameters (e.g., the size of a solar collector)
- Information parameters (e.g., a control algorithm)
- Decision parameters (e.g., the existence of a solar collector)

Decision parameters enable the user to take into account that certain elements of a component do not necessarily exist in every instance of the model. Decision parameters usually take the values true or false.

Concerning variables again a distinction between two kinds is made:

- Physical variables (e.g., temperatures, energies)
- Information variables (e.g., measured or set values)

Since the model is mainly designed for simulation of energy flows, special attention was paid to variables that characterize energy flows. This includes controlled energy flows and uncontrollable ones, such as waste heat as well as information variables linked to energy management strategies. In accordance with the reference model, the variable links between the components are shown in Figure 36 as thin black arrows. Every link can contain one or more variables.

Apart from the graphic representation and the general description of the model every component was represented in a textual manner in order to document the model in its entirety. A template based approach as proposed by the reference model was used to structure the component information similarly for all components. As an example the description of the component "Humans and appliances" is given in Table 1.

Table 3: Component specification template for the "Humans and appliances" component

HE

Humans and appliances

Physical Component

Executive summary

This part of the system describes the direct, measurable influence by the presence and activity of humans in the building and the appliances they operate in their sole discretion (e.g., computer, coffee maker).

Component description

This part of the system describes the direct, measurable influence by the presence and activity of humans in the building and the appliances they operate in their sole discretion (e.g., computer, coffee maker). Primarily this is the heat dissipation to the environment. Effects by influencing production machinery are not of interest in this component, only equipment, of which the operation mode can be controlled by the user is modeled by this component (especially PCs and displays, not central servers, which are described in PE).
This component only contains the physical model, i. e. the mapping of information concerning presence and behavior (activity, equipment use) supplied by HB (human behavior) to physical values.
Electric equipment of small power demand that is operating continuously (info displays, alarm systems...) is taken into account as a flat-rate value per square meter. People, cooking equipment and sanitary facilities, emit sensible as well as latent heat (humidity), other electric equipment emits only sensible heat. It is not distinguished between radiative and convective share.
Potentially effects on the indoor air quality could be modeled in this component. For reasons of complexity these effects are not taken into account.

Interface description

The component HE receives information concerning presence and behavior (activity, equipment use) supplied by HB.
The sensible and latent heat emitted by people and equipment of HE is injected into the thermal building model TBM. Information about the electricity demand of equipment is supplied to the energy system control aspects ESC.
The presence of humans furthermore influences the control of the lighting and thermal energy supply (LMC, TSC). TSC is furthermore informed about the water demand. In what way LMC and TSC are informed about this aspects in the real-world (manual handling, sensors) is part of the control strategy depicted in these components.

Parameters

Parameter name	Phys. unit
Nominal power of operable equipment 1_n-m_n in each thermal zone	W
Heat load of people in each zone	W
Nominal power of continuously operating devices in each zone	W/m²

	Evaporated water of people in each zone	kg/s
	Nominal water evaporation of equipment 1_n-m_n in each thermal zone	kg/s
Input Variables		
	From HB for each thermal zone	
	Number of present people	-
	Present clothing state of people	m²K/W
	Present physical activity of present people	-
	Present hot water use	kg/s

After fully determining and documenting the conceptual model, the simulation team started to derive the simulation model from the conceptual model, which represents the transition from the conceptual model to the implementation. Since the conceptual model was already designed with the aspect in mind that every component could be executed by one single simulation environment, this task simply consisted of uniting conceptual model components to simulation components and reducing the conceptual model interfaces to the interfaces that must be implemented. The result can be seen in Figure 37. Unsurprisingly, the choice of simulation environments and simulation model bundling coincided with the expertise in domains and domain specific environments assessed in the project initialization phase.

Since several different simulation environments were preferred by the experts it was decided to implement the simulation as a co-simulation. The reasonable choice of form of co-simulation was a loose coupling of Jacobi-type with a time step of 15 minutes between variable exchanges. The co-simulation was implemented using the simulation framework BCVTB, which is described in more detail in Chapter 2.5, because it corresponded well with the requirements and provided interfaces for all the used simulation environments.

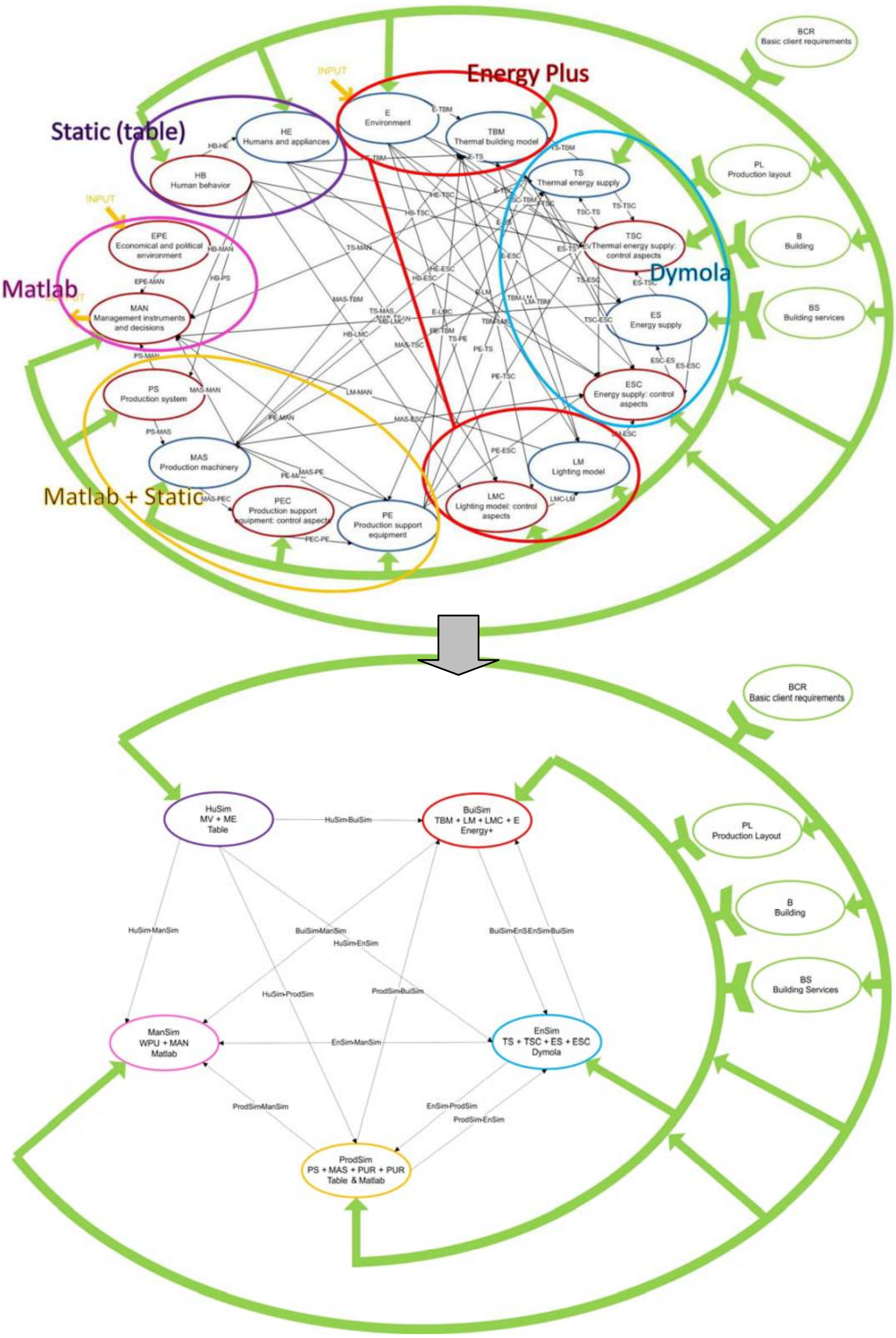

Figure 37: Reduction from conceptual model of production plants to simulation model

5.4. Sub-Model Energy System

The model of the energy system, which was composed of the component models “Energy system”, “Thermal energy system” and their respective control components as described above, depicts all energy conversion devices, storages, and energy consuming building service systems. The models of energy conversion units, storages and pumps were pulled from the model library described in Chapter 4.4. The components for the energy grid, that form energy balances had to be modeled according to the interfaces and demands of the specific application case. Therefore, the basic considerations leading to a functional energy system model shall be described briefly.

The energy demands of the other sub-models of the simulation (production, equipment, buildings) acts as an input for the energy system model and are processed by the models of the energy conversion until, at the end, the required final energy demand and the related CO_2 emissions are calculated and can both be used for further LCBA analysis.

In an intermediate step, the actual exergetic heat, cold or electricity demand needed to cover the room heating and cooling demands calculated in the building simulation are computed. In this step may occur a shift between types of energy because some of the required heating and cooling energy may be supplied as another type of energy (e.g. electricity instead of heat in case of use of small heat pumps) or covered by heat recovery (e.g. in the air-conditioning system).

Using the calculated heat and cold that needs to be transported in the lines of the system and the temperature difference between feed and return flow as well AS the supply air demand of the ventilation system, the mass flows to be transported in the lines are calculated. Using models for pumps and ventilators the energy demand for the distribution of the heat is determined. The total amount of electricity, heat and cold is calculated as the sum of the demand obtained directly from other components via model interfaces, the demand of the room conditioning system and the demand of the heat distribution system. The resulting total demand is than converted in the energy supply system in several steps until eventually results the final energy drawn from the grid. An overview of the resulting model architecture of the energy system submodel can be seen in Figure 38.

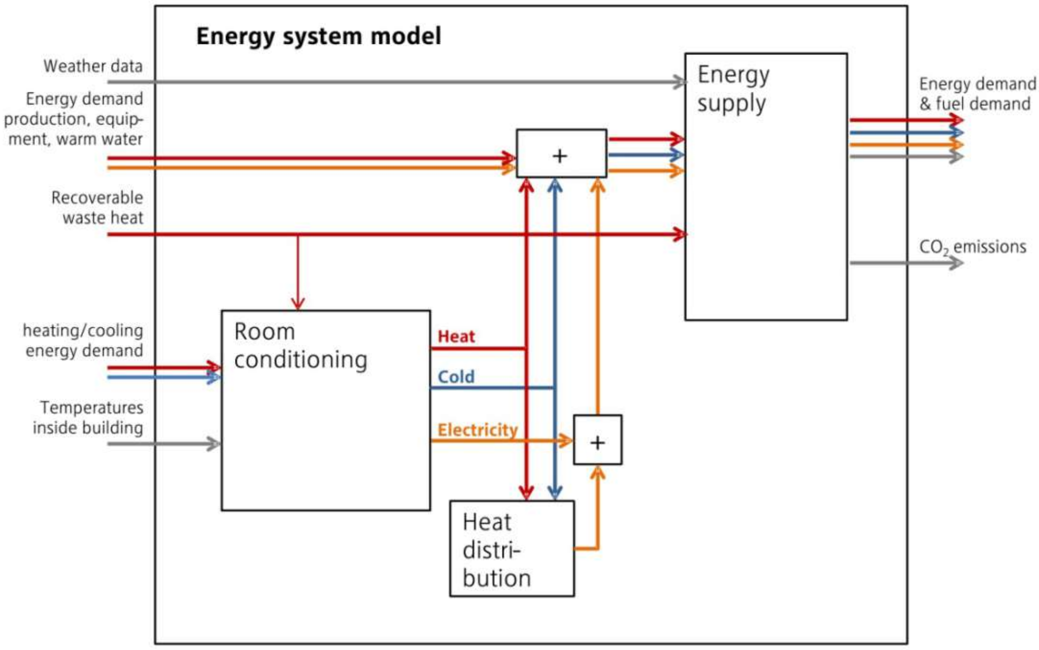

Figure 38: Architecture of energy system model

5.5. Validation and Verification

In order to ensure validity and credibility of the model several validation and verification techniques were applied on different levels of the model (top-level, submodel-level, component-level) and for the different development stages (conceptual and implementation). The validation also followed the top-down vs. bottom-up paradigm, by checking the top-level and the overall outputs of the submodels in a top-down approach, whereas the components of the submodel were validated and verified bottom-up. However, with the simulated system not available for final comparison of the simulation results to real-world data a certain uncertainty of the validity of the results remains.

Since the model was derived from the system understanding or knowledge about the system in a deductive manner, the top-level conceptual model validation was concentrated on the logical and structural validity. Due to lack of results that could be compared to data about the system, the validation relied on comparing the model to mental knowledge about the system, provided by the experts in the team. Also during the validation process the relatively diverse simulation team in terms of expertise made it possible to always have models checked by simulation team members who were not involved in their respective development. The validation techniques applied were mainly informal techniques such as checking and face validation (see Chapter 3.4). Furthermore, the graphical representation proofed to be very helpful to track the consistency of data flows through the model.

For the energy system sub-model at top-level the conceptual model was critically reviewed by the developer and during the implementation more formal techniques for V&V such as symbolic execution, path analysis and assertion checking were applied. All the component models were subjected to static analysis in terms of semantic analysis, consistency checking and of course syntactic analysis by compilation. Furthermore, symbolic executions were performed with all of the models. If useful parameterization, input and output data for comparison could be found (e.g. from manufacturer data) black box tests were executed. However, these tests do not say anything about the validity of the input data. Since the data for parameterization of the energy system components was mainly derived from manufacturer specifications and no information about performance under real operating conditions was available, the operational validity of the models cannot be determined completely.

In the end the results of the completely assembled simulation model, including all submodels were thoroughly reviewed by several members of the simulation team in terms of consistency and plausibility of the obtained results. Furthermore, certain key parameters (such as annual heating demand per square meter) were compared to expected values under similar condition. Anyhow, operational validity can only be assured completely by comparing simulation results to real system. So if the real system does not exist like in this case, the model results should be considered rather as qualitative indicators then quantitatively precise predictions. A sensitivity analysis could have helped to gain credibility by determining the impact of flawed data of singular components on the overall system behavior, but was unfortunately not feasible within the project to the desired extend, due to lack of resources.

5.6. Case Study

As required by the project proposal in the end of the project a cases study was to be conducted as a proof of concept of the simulation tool. In order to identify which parameters have determining effect on the system behavior in terms of energy demand a series of preliminary analysis with more or less generic simulations were conducted. Studies concerning buildings and the production system were published by consortium members in [143]. The study concerning the energy system shall be presented here.

The simulation consisted of models for the production, the building and different HVAC system, which were compared concerning heating and cooling energy demand depending on location and degree of capacity utilization. The aim of the generic simulation was to get an idea of the performance of certain energy supply systems under different influences concerning climate and production scenarios, especially with focus on cooling and waste heat reuse.

Three different scenarios for the capacity utilization (low, average, high) were generated based on measurement data. The energy used by the production was injected into the building model. This model calculated the heating and cooling energy demand necessary to maintain certain comfort conditions within the building based on the waste heat from the production and weather data of three different locations. The energy supply was covered by two different building energy systems. In the "conservative" scenario the heating demand was covered by an oil fired heater and the cooling energy was supplied by a compression chiller. From it resulted the electricity demand for the cooling and the heating demand, which was calculated from the oil demand by multiplying with the calorific value. In scenario two the heat demand was covered by a heat pump, which used ground water (10°C year around) as a heat source. The cooling was realized by an absorption chiller, which reused waste heat from the production and the remaining heat demand was supplied by a third party (e.g. district heat). Therefore, scenario two ultimately calculated the electricity demand, which was used for heating and the heat demand supplied by external providers for cooling purposes.

Three selected days during the year (winter, spring, summer) were simulated with climate data from three different locations (Cairo, Vienna, Moscow). Table 4: Parameterization of key parameter analysis shows an overview of the simulation parameters.

Table 4: Parameterization of key parameter analysis

Production					
Capacity utilization low	680.97	kWh	Injection time	8:00 - 18:00	
Capacity utilization medium	1361.94	kWh			
Capacity utilization high	2042.92	kWh			
Building					
Length (north-south)	74	m	U-factor outside walls	0.35	W/(m² K)
Width (east-west)	50	m	U-factor roof	0.16	W/(m² K)
Height	12	m	U-factor floor	0.3	W/(m² K)
Temperature set-point heating	20	°C	Glazing	10 - 20	%
Temperature set-point cooling	26	°C	Thermal zones	5	
Building services					
Scenario 1			Scenario 2		
Oil heating nominal power	380	kW	Heat pump nominal power	380	kW
Oli heating efficiency	0.93		Absorption chiller nominal power	4 x 62.5	kW
Compression chiller nominal power	250	kW	Heat recovered from production (% of electricity consumed)	40	%

The results of the simulation are shown qualitatively in Figure 39, Figure 40 and Figure 41. It is evident, that the heating power supply can be provided more efficiently by the heat pump than by the oil heating. The absorption chiller has a higher energy demand than the compression chiller. Scenario two therefore is to be preferred in colder climates since it operates with lower energy consumption than in warmer climates. In warmer climates (Cairo), the absorption chiller is preferable to the compression chiller only with support by additional heat sources, e.g. a solar thermal system.

Furthermore, it can be observed that starting at a certain level of capacity utilization of the production the externally supplied heat demand ceases to increase because the internally supplied waste heat covers the demand. Overall scenario two shows a higher efficiency at higher capacity utilization than at lower utilization due to the waste heat reuse.

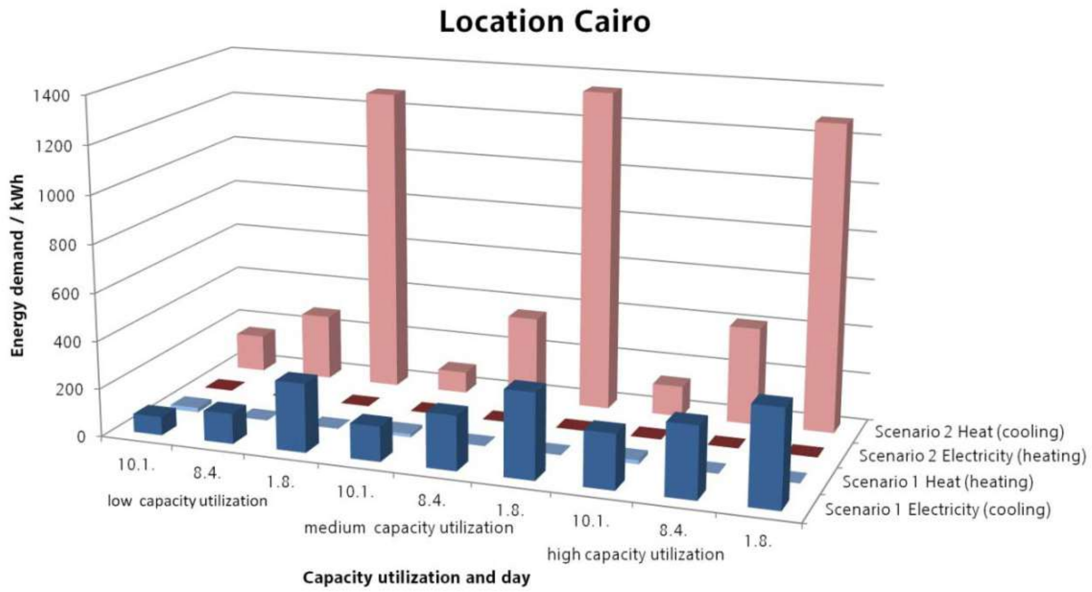

Figure 39: Results of key parameter analysis - location Cairo

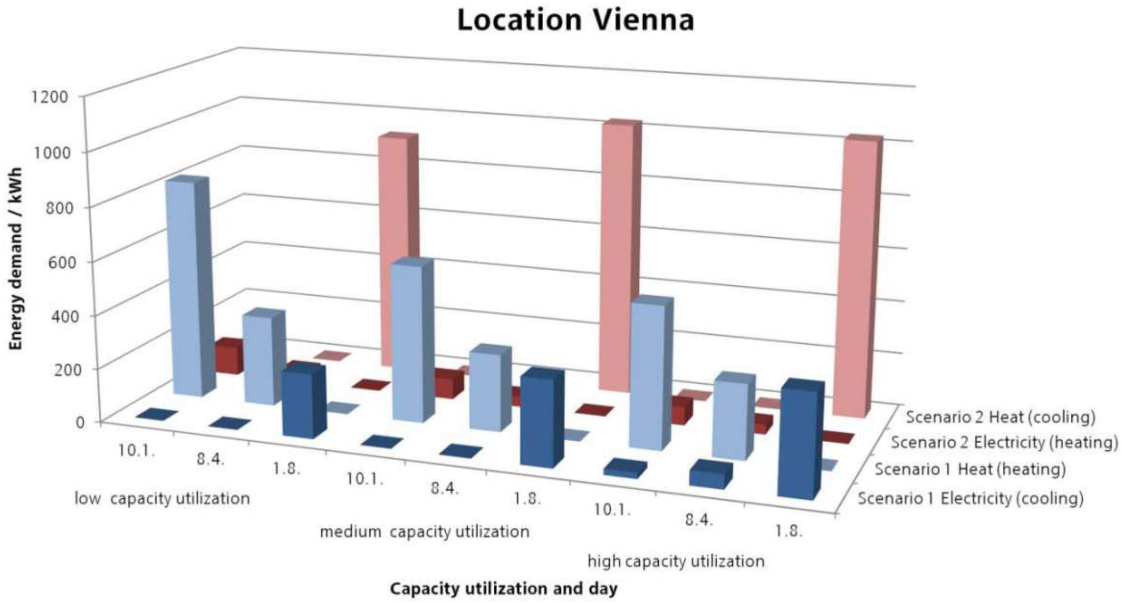

Figure 40: Results of key parameter analysis - location Vienna

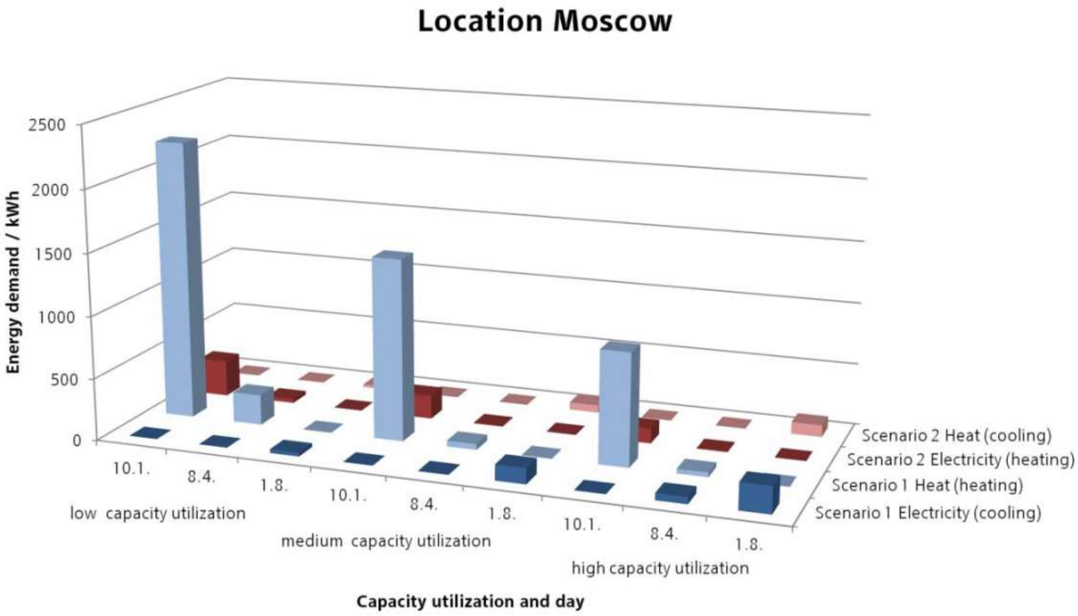

Figure 41: Results of key parameter analysis - location Moscow

The simulation results clearly show that the efficiency of an energy system in an industrial enterprise is strongly dictated by the climatic and production-related conditions. The exact matching of the design of a building or building equipment to the usage scenarios is difficult to achieve due to considerations of flexibility, therefore it is important to find energy systems that can adapt to the different scenarios with the highest possible flexibility. Under consideration of these results in one scenario of the case study absorption chillers were integrated to cover the heat demand.

The case study was carried out as a proof of concept for the co-simulation tool and represents a specific instance of manufacturing companies that can be modeled and simulated with the developed tools. As planned in the implementation phase, models are executed using different simulators and the integration of the models was realized with BCVTB.

As a reference object the production facility of a consortium member, who planned to move the production to a new location, was chosen. At the time of the project the company conveniently was at the beginning of the planning process, so the ideal point in time to apply the simulation tool as planning support was given. The respective company performs metal cutting processes for small batch production and moves to a new building, keeping the existing production equipment. The company has approx. 500 employees, a machine park of 48 machines and an annual energy demand of close to 8 Mio. kWh.

The new building for which a concept was developed during the preliminary studies should unite the demands of energy efficiency and flexibility of layout and structure. It features 20.500 m^2 production area and 15.000 m^2 office and representative area. Through previous simulation of nine scenarios varying several parameters, the best scenario in terms of heating and cooling energy demand could be identified, to enter the integrated simulation. Optimized air exchange rates (winter: low, summer: high) paired with automated lighting and shading reduces the heating demand by 50%, and the cooling demand by 20%. [143]. The model of the described building was integrated into the simulation in the component BuiSim and implemented in the simulation environment EnergyPlus (see Figure 37).

The machine park, consisting of machine tools, ovens and laser cutting machines, was mapped in a data-based model. Thereby, data from the production planning system, such as machining-time and set-up time of individual production jobs on specific machines were used to specify the operational state of the machines. Typical values for cutting-parameters were derived from measurements during machining of typical work pieces on site. As a next step the compressed air consumption of the production was analyzed and modeled. The electrical power of the compressors was determined using a physical model based on ideal adiabatic compression. The machine park is found in the component ProdSim in the simulation model (Figure 37) and was technically implemented as a static table interfaced into BCVTB via Matlab.

Finally three different energy systems were compared in order to find the most suitable alternative for the proposed production and building. The energy systems correspond with the component EnSim in the simulation model and were implemented in Modelica and executed with Dymola. The three compared systems differ mainly in the form of the energy (heat, cold, electricity) supply. An overview of the three variations can be seen in Figure 43, Figure 45 and Figure 47. They shall be discussed in more detail below and furthermore the results of the simulation study are shown as Sankey diagrams and as comparison of the total demands and emissions. However, since the result values could not be validated and no sensitivity analysis was conducted, the results should be regarded rather as qualitative indicators of certain phenomena than reliable quantities. Therefore, no numerical values are provided.

For the transfer of heat or cold into the rooms the following systems have been planned for all three variants:

- Displacement ventilation in the production area
- Ventilation via a raised floor in the offices
- Ventilation ceilings and displacement ventilation in the ancillary spaces, kitchen, canteen etc.
- Ceiling mounted radiant panels in the production
- Underfloor heating and cooling in the ancillary spaces, kitchen, canteen etc.
- Small heat pumps in the offices

With the exception of the small heat pumps and the ventilation, the type of injection is secondary for the energy system simulation. This is due to the fact, that only the energy flows were relevant for the simulation, not the thermal comfort condition in the rooms and therefore no modeling of the exact nature of the injection was necessary, with the exception of ventilation due to the heat recovery, and the small heat pumps, in which a conversion of energy forms (heat/cold to electricity) takes place.

In the system variations 1 and 3, the production hall ventilation is designed as a compact supply and exhaust air unit with heat recovery. For this purpose, heat pumps with a total nominal thermal power of 770 kW would be installed in the exhaust air device which would deprive the entire thermal energy from the exhaust air and supply it to the low-temperature line. Thus there is no direct exchange between the fresh air and the exhaust air. Water-bound transport of energy is more efficient and especially with the installed heat pumps a highly efficient heat recovery. The disadvantage is certainly the increased demand for electricity in the heat recovery, which must be compared to the savings in heating power.

In variation 2 a rotary heat exchanger (heat recovery level 75%) is used. Since the exchanger cannot cover the entire heat demand for the preheating of the inlet air form the exhaust air, additional heating must be applied.

This effect can clearly be observed in the simulation results. The electrical power consumption of the HVAC in variation 1 and 3 is significantly higher than in variation 2, while the thermal energy demand for room conditioning is larger in variation 2 (see Figure 44, Figure 46 and Figure 48).

The hot water generation is carried out in the same way in all three versions. 50 m² of solar thermal collectors in southern orientation and with 20° inclination are provided. A buffer tank of 3000 liters is used for storage. The remaining hot water demand is met by means of an electric heater. The simulation confirmed the planning assumption that this system should be able to achieve a solar fraction of 25% of hot water generation. In all three variations a south facing photovoltaic system of 2500 m² on the rooftop, with an angle of inclination of 20 ° is planned.

Apart from the aforementioned characteristics the form of energy supply is fundamentally different in the three variations.

In variation 1 (overview see Figure 43) two natural gas-fired cogeneration plants and four absorption chillers are used. The CHP plants produce electricity and heat which can be used for heating and operating the absorption chillers. With respect to the thermal power supply of the heating and the chiller, the CHP units are designed for 6000 hours of full load annually. Therefore, they are operated heat-controlled. The nominal electrical power of the units is 1165 kW and the nominal thermal power 768 kW at a power consumption of 2926 kW. The advantage of the cogeneration plant is that natural gas has much lower primary energy conversion factors than electricity i.e. in terms of the primary energy demand the CHP shows a better performance than concerning the final energy demand. The drawback is the relatively low efficiency, especially at part load. The peak loads of the heat demand are covered via district heating.

The absorption chillers use the heat produced by the CHP or waste heat from the compressors of the production. Due to the operation mode of the absorption chiller (also see Chapter 4.4.1), it demands a very limited amount of electrical energy to realize the compression, but heat at a temperature level of about 80°C is needed. The only facility internal heat recovery that provides a sufficient temperature level, are the pressurized air compressors. Disadvantages of the absorption chiller as opposed to the electrically powered compression chiller are, first, the low part-load capability and second the relatively high energy consumption resulting in a low COP. Advantage is the substitution of high exergy electricity with heat as an energy form of lower exergy. The four absorption chillers each have a nominal cooling capacity of 625 kW and demand 875 kW of heat flow input. By throttling of the heating water mass flow a part load state of about 75% of the nominal capacity can be achieved.

The negative impact of limited part-load operability of the absorption chiller immediately becomes apparent when reviewing the simulation results of variation 1 in more detail (see Figure 42). It exemplarily shows the profile of required cold demand of hall and office and the heat production of the CHP plant and the recovered waste heat from the compressors in a summer week i.e. the in- and output of the absorption chillers. A massive amount of heat input, delivered from the CHP and the heat recovery is needed in order to cover a relatively low cooling demand from the production. This is not due to the low efficiency of the chiller (in the design point the COP is about 0.71), but to the low power requirement, which is often in a part load range which the machine cannot reach i.e. it is oversized and a large portion of the produced cold cannot be used. This effect is also the cause of the eye catching shape of the simulation results for the produced heat. The heat generation does not follow the demands, but extends stepwise. The steps mark the respective power limits of the absorption chillers. Furthermore, the CHP units are designed relatively generously and therefore operate mainly in part load range with poor efficiency. Due to the characteristic that the cogeneration unit is operated heat controlled, it also creates an electricity overproduction, which has to be supplied to the grid. This effect is even more prominent in the colder months of the year, when the cold demand and the smallest possible amount of production deviate even more.

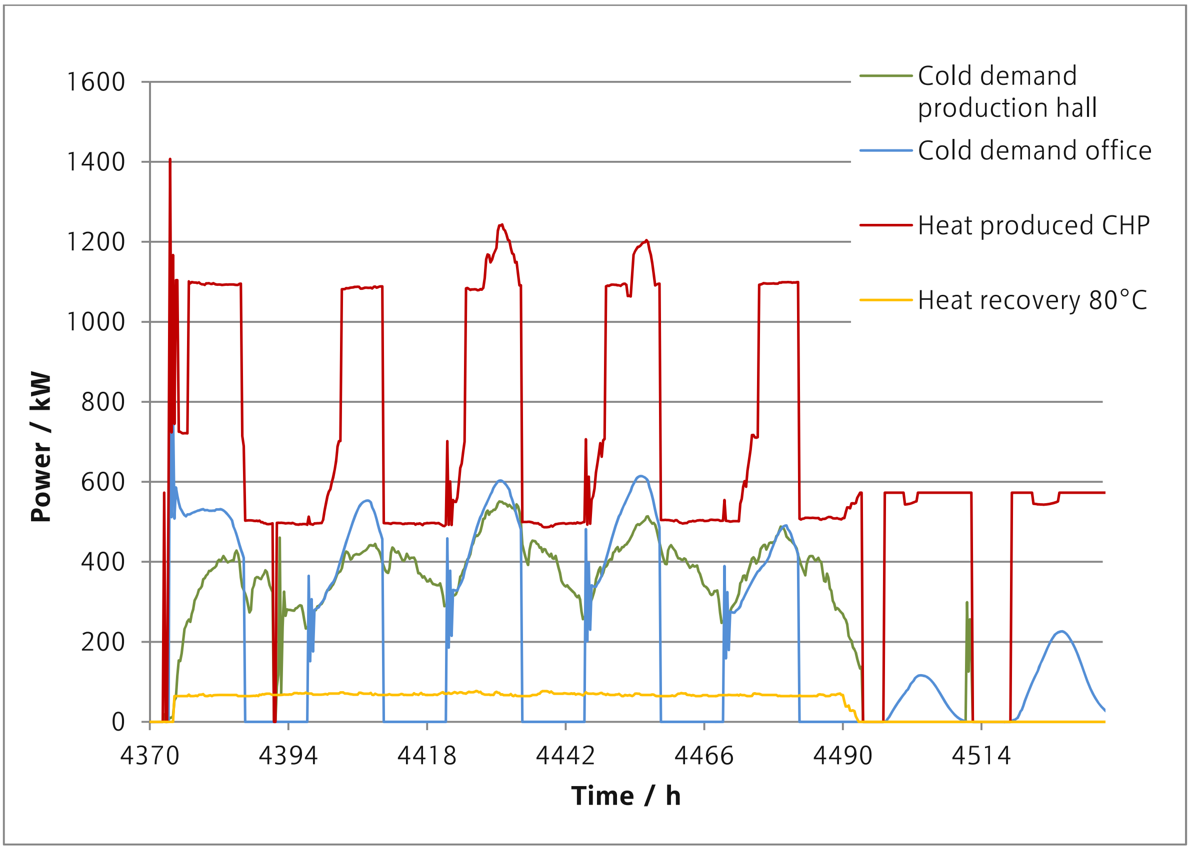

Figure 42: Correlation between cold demand and heat production in a summer week

Remedy could be created by installing sufficiently large buffer storages. An alternative would be the installation of smaller, but more units. In any case, it is clearly evident that the wrong design of the machines can have a significant negative impact on the energy efficiency.

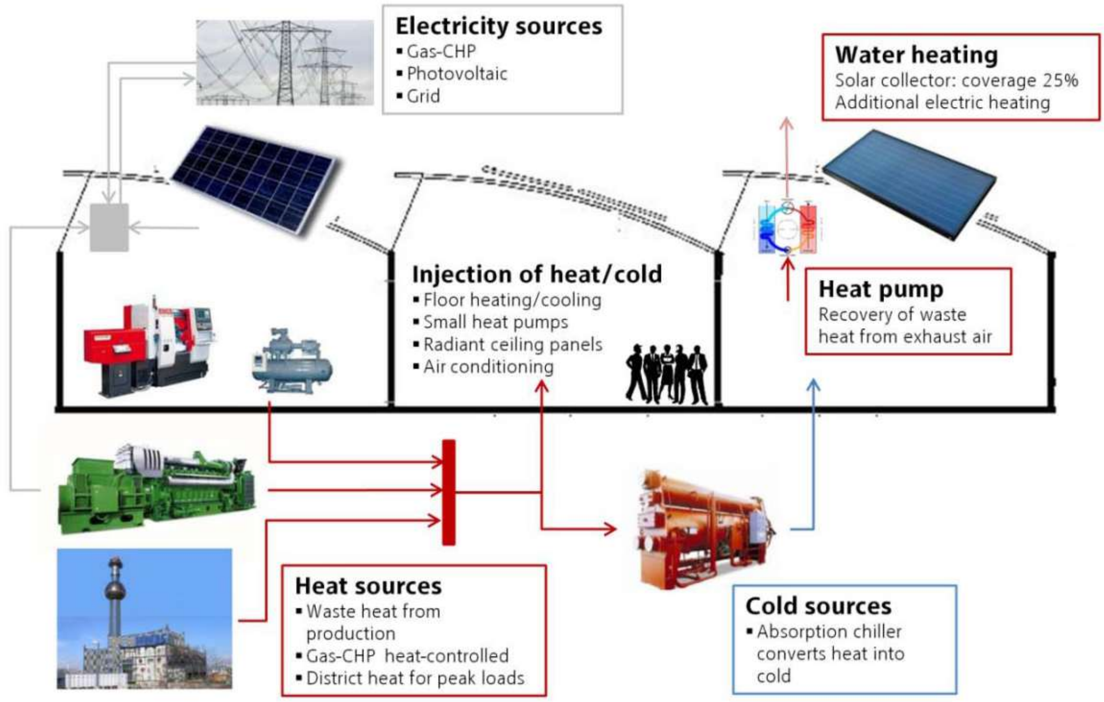

Figure 43: Overview of energy supply system variation 1

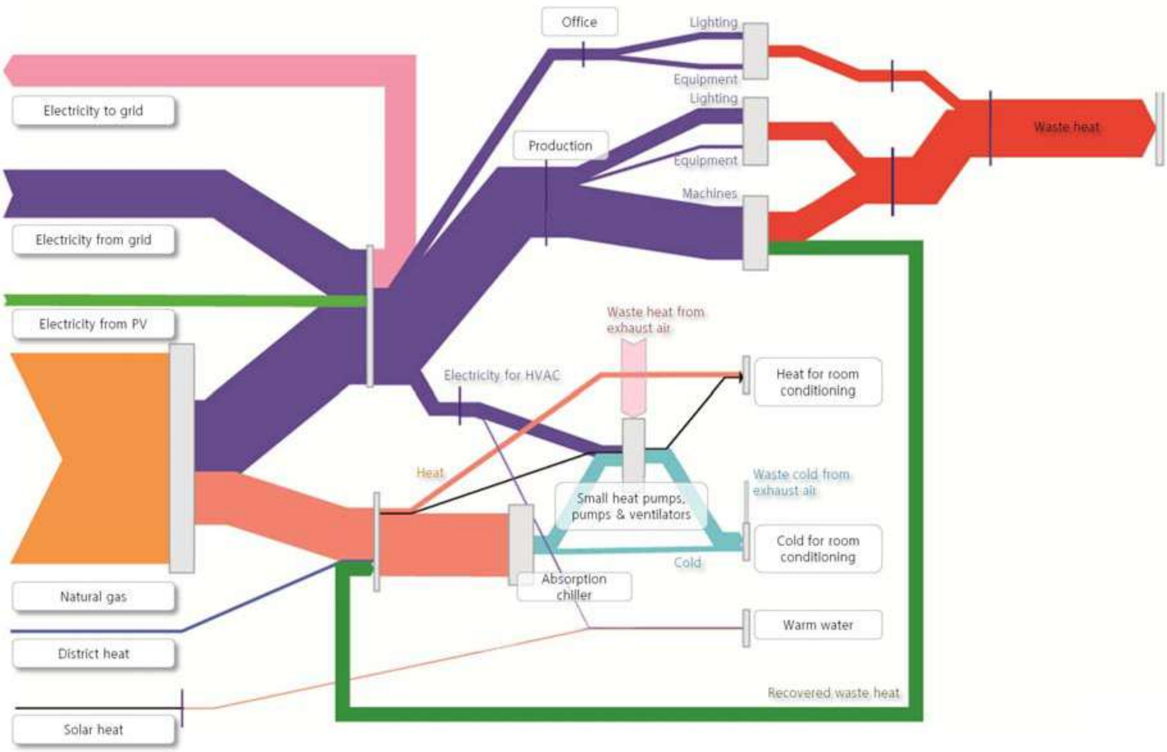

Figure 44: Qualitative simulation results of energy supply system variation 1

In variation 2, the heat required is supplied exclusively by district heating. The cold is provided by electricity powered compression chillers (two times 1200 kW) (see Figure 45). The simulation results, depicted in Figure 46, show that much less energy for cooling is needed than in variation 1, since the compression chiller has a much better COP than the absorption chiller. In return energy of higher exergy and therefore higher price must be used. It can also be recognized that the reused waste heat from the production is considerably lower than in the first variation. This is due to the fact that the heat can only be reused if use and demand coincide in time (if no thermal heat storage exists). In variation 1 waste heat can be reused for heating and cooling purposes, so possibilities of use expand over the course of the whole meteorological year, while in variation 2 heating is the only option. Moreover the electricity and heat demand of the HVAC system differs, as already mentioned, due to the different heat recovery concepts.

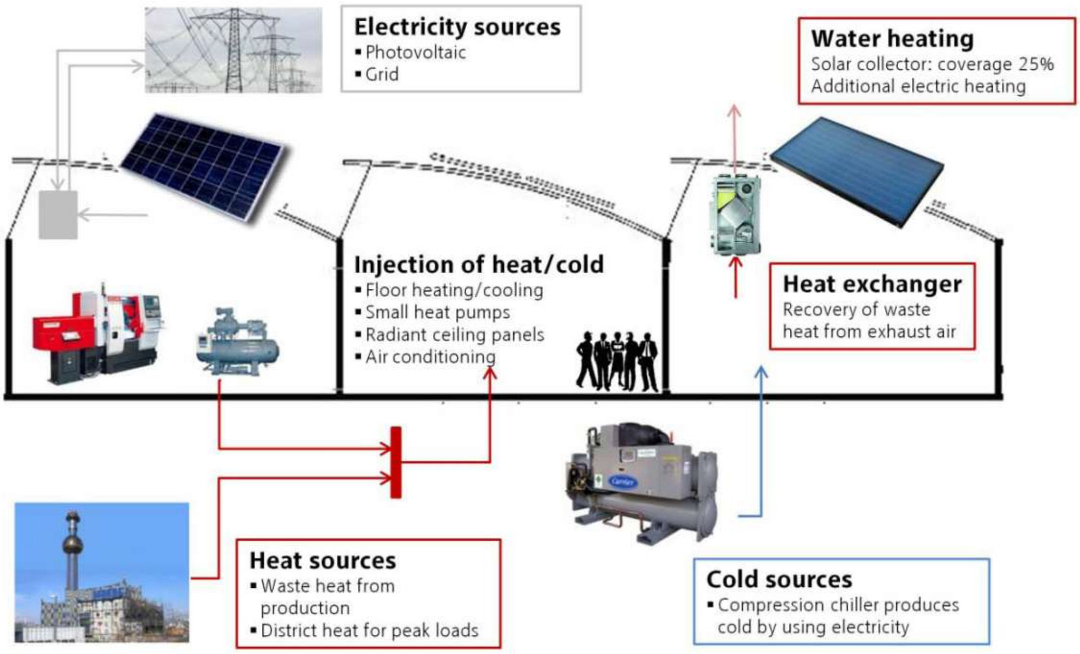

Figure 45: Overview of energy supply system variation 2

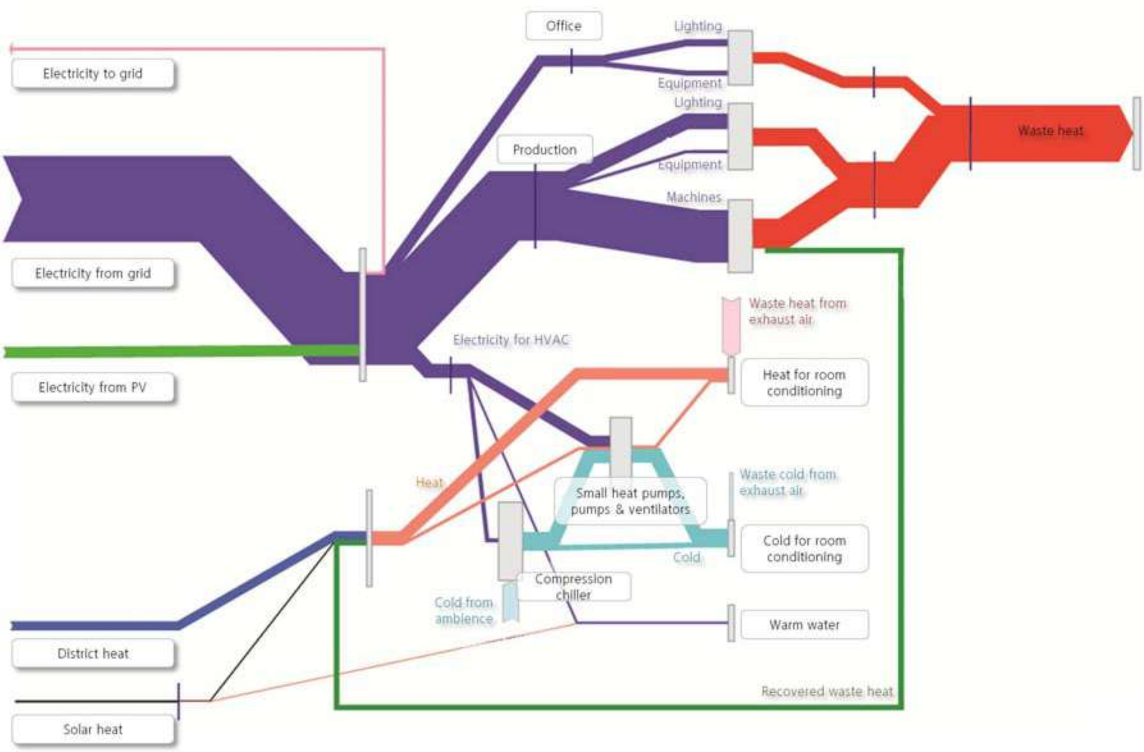

Figure 46: Qualitative simulation results of energy supply system variation 2

In version 3, the required heating and cooling energy is supplied from a groundwater well (see Figure 47). The heat is then transferred to the desired temperature level by means of a heat pump (3000 kW nominal thermal capacity). The heat pump is designed generously, since no back-up by district heating is provided. A chiller is not required because the temperature of the ground water is sufficiently low for room conditioning purposes and therefore can be used directly.

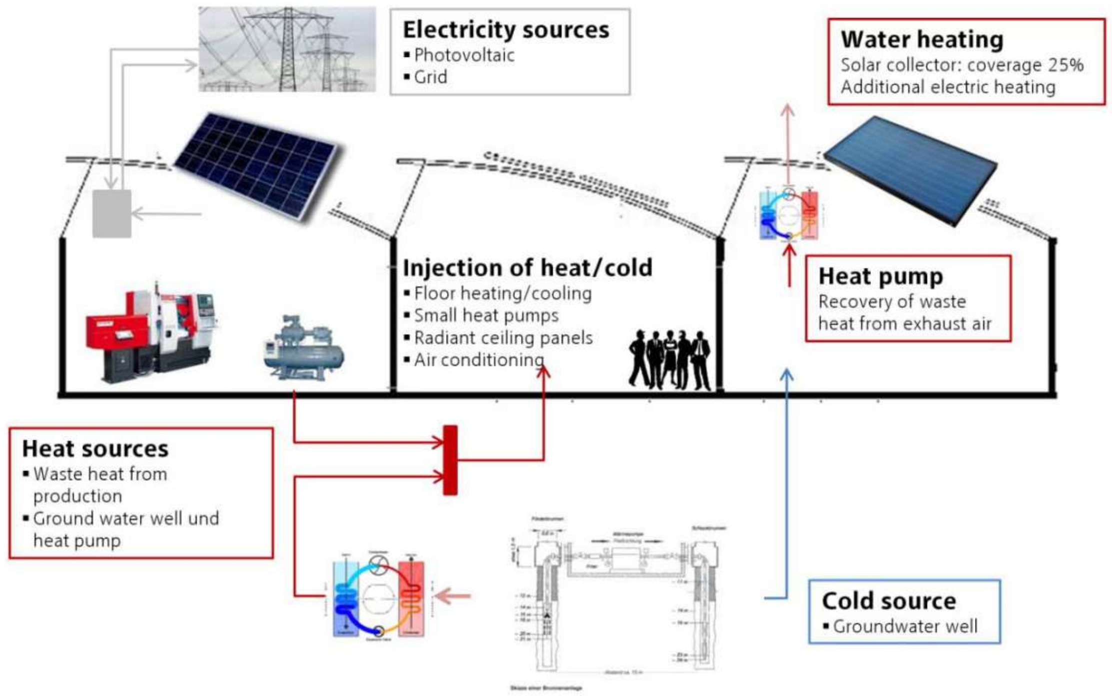

Figure 47: Overview of energy supply system variation 3

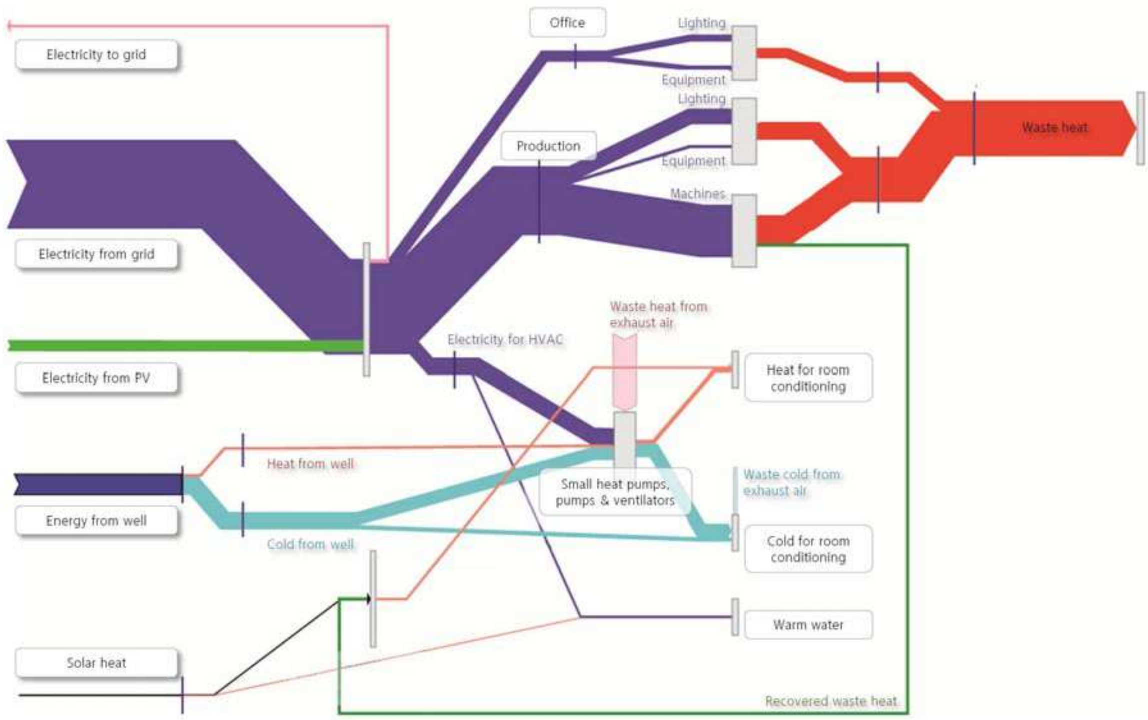

Figure 48: Qualitative simulation results of energy supply system variation 3

Of course, scenario 3 turns out to be favorable because the energy from groundwater is available for “free”. However, due to the relatively limited groundwater availability it cannot be considered entirely unproblematic. If groundwater is used by everyone (at the same time) as a heat source or sink, problems can result, especially in highly populated urban areas. Furthermore, it should be noted that a certain temperature difference between extraction and injection wells must not be exceeded. Evaluation of the simulation results also showed that the heat pump and the operation of the groundwater well pump cause additional power consumption.

Comparing the variations in terms of energy consumption, it is immediately apparent that variation 1, due to the problems in design, is significantly inferior to scenarios 2 and 3 in terms of final energy demand (Figure 49) and also worse than the historical consumption data of the old plant, although initially it was expected to be the most efficient variation. This slightly levels out for the primary energy demand and CO_2 emissions (Figure 50), since scenario 1 has a lower electrical power import from the grid, because for electricity generation in the CHP natural gas is used instead, which has much lower primary energy and emission conversion factors compared to electricity, according to the guideline in effect in 2013, when the analysis was carried out [144]. Options 2 and 3 have approximately equal consumptions and emissions, but the above mentioned groundwater problem remains for version 3. Also, it must be mentioned that the present result is valid for the location Vienna and the conversion factors applicable to the Vienna district heating and may differ at other locations.

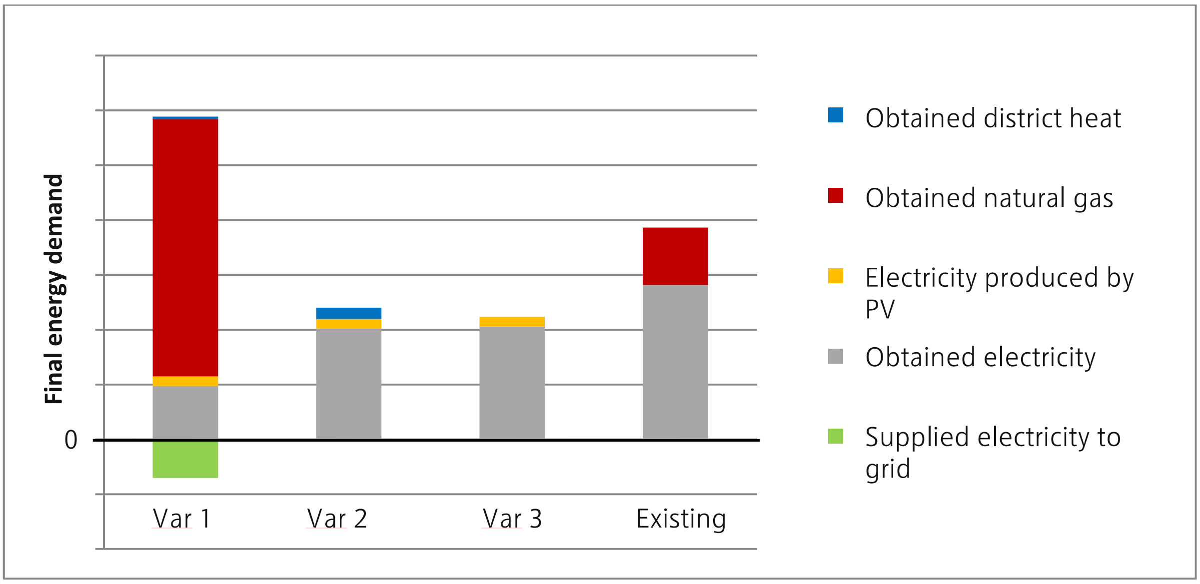

Figure 49: Final energy demand of existing plant and 3 simulated variations

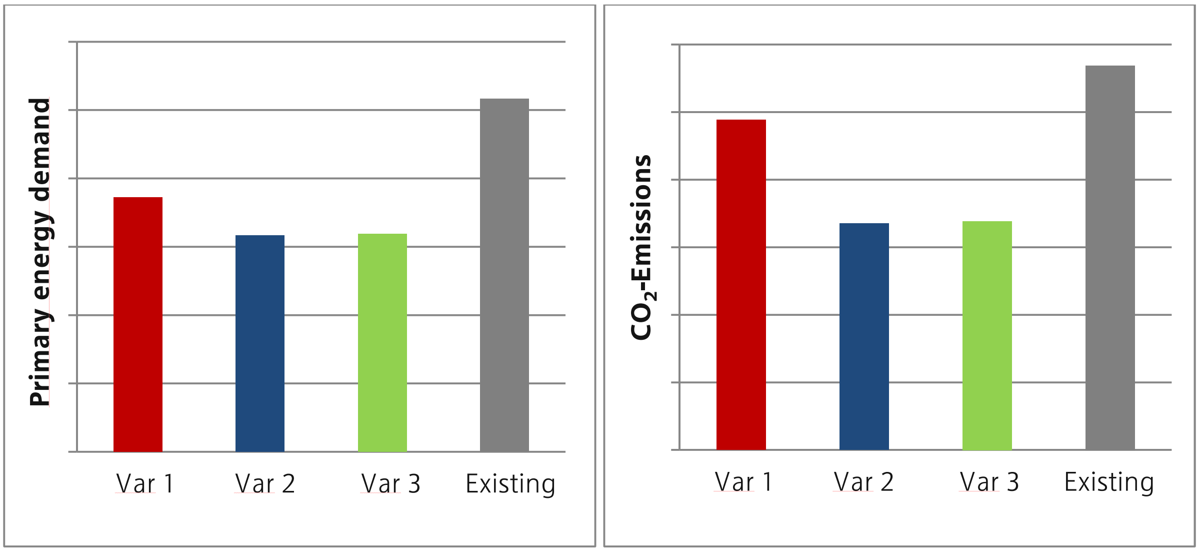

Figure 50: Primary energy demand and CO2 emissions

The results shown were finally processed by the economic expert group into significant performance indicators. Investment, maintenance and energy costs were taken into account when calculating the expected cost-benefit relations. After a life cycle period of 30 years variation 2 caused about 6% less costs than variation 1 and variation 3 8%.

As a conclusion of the preliminary study and the case study a number of key influential parameters on the energy performance of production plants could be identified as foolws.

Type of equipment used

The coordination of building systems and the type and volume of production processes have a strong influence on the efficiency of the energy system. Above all it must be ensured that plants, reusing energy from other processes, are designed to match the offer. Under certain circumstances it can be reasonable to cover additional demand by other types of energy conversion systems (absorption- vs. compression chiller resp. hybrid solutions). The use of different energy sources also creates flexibility to react to changing conditions.

Dimensioning of the equipment

Many energy systems operate relatively inefficiently outside their design point and posses a limited capability to operate in partial load. Therefore it is important, to adjust the equipment as closely as possible to the demand and provide several smaller units rather than one large one. Again, solutions based on the use of several different energy sources, provide efficient solutions. Alternatively the application of sufficient storage potentials can be advised.

Temperature levels of the system

Careful assessment and selection of the energy system's temperature levels has great impact on the efficiency of the system. Generally it is necessary to recover waste heat at a temperature as high as possible and to maintain it. Again, this has to be matched with the demand. High temperature waste heat, which cannot be utilized, does not make the system more efficient. Under certain circumstances it is also possible to raise the temperature by a few degrees by means of a heat pump.

Temporal availability and demand

In addition, waste heat recovery goes in vain if no use can be made of it. It is therefore important to adjust the sources with the options of use as well as the temporal availability. Cold production by heat (absorption / adsorption chiller, sorption) extends the usability period of waste heat from the heating to the cooling period or process heat to process cold.

6. Application Case Model Predictive Control of a Building

6.1. General Project Description an Initialization Phase

The project SmartCityGrid:CoOpt (CoOpt) was established in 2012 and completed in 2015. The project goal was to maximize the coverage of the energy demand of urbanized areas by renewable energy sources. Previous investigations of project partners had demonstrated that in an urbanized city district 100% coverage of the electrical energy demand by means of renewable but fluctuating energy sources over the year is in principle possible. However, due to temporal distribution of demand and supply and technical restrictions of the existing urban electric energy system self coverage is limited [15]. Storage systems can only counteract this problem to a certain extent. So, in order to reach a global optimum in the sense of direct utilization of renewable energy and energy efficiency, the overall electric distribution network in context with the supplied buildings must be considered. In this context Demand Side Management (DSM) plays an important role. Palensky and Dietrich define DSM as:

> *Demand Side Management (DSM) is a portfolio of measures to improve the energy system at the side of consumption. It ranges from improving energy efficiency by using better materials, over smart energy tariffs with incentives for certain consumption patterns, up to sophisticated real-time control of distributed energy resources.* [87]

DSM is not limited to saving energy (although energy efficiency is a part of DSM), but also includes measures to influence consumption patterns, in order to achieve a temporal harmonization of demand and supply. This is mainly achieved by load shifting and peak shaving. A key requirement to successfully apply these techniques is of course sufficient storage potential. A number of studies have assessed the potential of different kinds of thermal storages [74], [145]–[147]. But other prerequisites are necessary as well. Strbac analyzed that lack of ICT infrastructure (advanced metering, communications, control methods), lack of understanding of DSM benefits and increased system complexity inhibit the application of DSM technologies [148].

In order to gain more insight into the topic and to develop a global systemic energy management at the levels of the building and the distribution network the project SmartCityGrid:CoOpt was initiated. The project set out to achieve this goal by realizing load shift potentials through an optimized use and integration of thermal and electrical storages and passive storage masses in buildings into the urban energy management. To realize this, a methodology for optimized control strategies, based on model-predictive controllers (MPC), was proposed. The project focused not only on the building. In order to realize a global systemic optimization, a hierarchical control concept, containing a building controller on the lower level and a grid controller, was developed.

The two optimization levels (building and grid) were to be developed separately and linked in the final stage of the project, in order to achieve a holistic methodological approach, Furthermore, strategies for an overall systemic, coordinated optimization were promised in the proposal. While the optimization of the building was to be demonstrated by hardware-in-the-loop (HIL) integration of a real building, the optimization on grid level stayed of theoretical nature, demonstrating the achievable benefits via simulation.

The building chosen as a reference case was an office building and incorporated major thermal storage potentials. Exact models and predictions, related to the development of demand, production, and consumption or weather related forecasts, were to be assembled with the actual predictive control algorithm into a simulation framework and later on into a hardware-in-the-loop application with the real building.

The chosen methodological approach of the project also picked up major research trends in building performance modeling, like simulation assisted control and computation time reduction for real-time applications (see Chapter 2.4), and to some extent prove their feasibility.

Due to the design of the proposal this application case significantly differs from the case presented in the previous chapter. The project INFO aimed at providing a universally applicable tool, which can be used to model and simulate most kinds of production facilities, which was only specified to depict one instance in order to proof the concept. Its intended use furthermore aimed at a quite conventional form of M&S application: analysis and comparison of scenarios. CoOpt was targeted at a very specific instance, with the object to be modeled known from the beginning, but the intended use in a real-time application, raised other challenges.

Due to the two levels of optimization the M&S tasks actually splits in two separated tasks. This chapter is mainly dedicated to efforts on building level, since the author of this thesis was only involved in this particular modeling task, but in Chapter 6.3 the link between the two systems will be discussed briefly, in order to give an idea about the connection between the two systems.

The part of the consortium involved in the building simulation and control integration included an interdisciplinary team of experts in control theory, building science and energy systems and an automation solutions provider. Concerning a detailed role definition the following expectations and expertises could be defined:

- Stakeholders. Three basic groups of stakeholders could be defined:
    - Funding agency (simulation sponsor) (1) has an interest in obtaining a valid, applicable tool with reuse value.
    - Facility management (2): The facility management of the building chosen as a reference object represents probably the most important stakeholder, since it can be seen as the representative of the building users, who are naturally interested in a flawlessly operating control to provide comfort in the building. Furthermore, it must be relied on in order to actually apply the designed control strategy. By design of the proposal, the facility management was not part of the project; a circumstance which proofed to be troublesome in the phase of implementation of the HIL application, because the cooperation was a matter of goodwill.
    - Simulation result users (3): The users of the simulation results mainly consisted of the grid controller M&S team and other researchers relying on the simulation results to carry out analysis concerning economic feasibility. Both had an interest in valid simulation results.
- Domain Experts. Three groups of experts were represented in the simulation team, all of which possessed proficiency in M&S related to their specific domain as well:
    - Building and energy system expert group 1 (4) contributed expertise considering the design of the building and its service systems and their simulation. Furthermore, they were residents in the reference building and had conducted previous research with the building as their subject of study. Therefore they possessed an in depth knowledge about it.
    - Building and energy system expert group 2 (5) contributed expertise considering the design of the building and its service systems and their simulation, especially

in interdisciplinary teams. This team had no whatsoever knowledge about the modeled object and had to rely entirely on information provided by team 1.
   - Control theory experts (6) were experienced researchers in terms of all aspects of control theory and highly proficient in related M&S methods and tools.
   - Automation solutions provider (7) contributed knowledge concerning the interface design to integrate the simulation into the building automation system.
- Simulation experts: The first three groups of domain experts also possessed expertise in M&S techniques of their specific domain.

The two building and energy system expert groups preferred M&S with Dymola/Modelica and the control theory experts used Matlab. Altogether, the roles in the project can be mapped as shown in Figure 51.

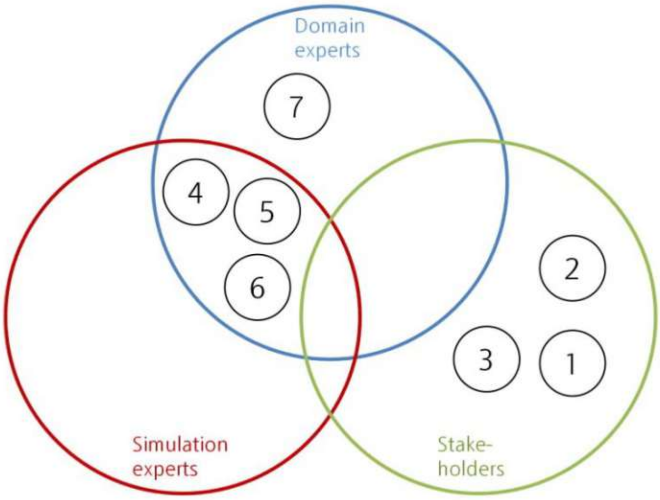

Figure 51: Role definition CoOpt project

6.2. Problem Formulation and Requirement Definition

The problem formulation and requirement definition in the CoOpt project was a considerably faster and more efficient process than in INFO. This is mainly due to the facts that the objectives and the system were already predetermined to a large extent by the proposal, that the task at hand was very concrete, that the M&S team had a more uniform approach to modeling and simulation, and at this point already possessed more experience in interdisciplinary cooperation.

Objectives and restrictions of the model:

Based on the proposal and a short discussion process the objectives of the building model and the connection to the grid model were formulated by the M&S team:

Objective of the model is to serve as a basis for the simulation of buildings and their respective energy systems as well as the electrical grid in which the buildings and their energy systems are integrated as consumers and producers. Of special interest within the simulation is the system's answer to different control strategies, especially model predictive control (MPC).

The two main fields of interest of the simulation, the building and the grid are simulated independently, in order to simplify the technical execution of the simulation. This approach does not take into account possible dynamic dependencies between the two *simulations. However, constraints impressed by the respective other part of the system are taken into account in the design of the MPC components. With this approach also the necessity of duplicating certain parts of the model arises.*

Substitution of certain components of the model by existing hardware in order to execute a simulation with hardware in the loop should be possible.[149]

Based on this relatively generic formulation of the objectives the object under study (the building) was analyzed in more detail.

System description and data and information collection

The building chosen as a reference object was the *Energy Base*, an office building located in Vienna, which offers about 5000 m² office space. The building was chosen for several reasons: The consortium leader is a resident of the building and already had conducted research projects about the building previous to the project. Therefore, the building was considerably well documented. Furthermore, the building is built at passive house standard and features an innovative building service design as well as large thermally activated buildings systems (TABS). These design features made it ideally suited to apply load shift strategies successfully.

Figure 52: Energy Base (picture source: bauinfo24.de)

Figure 53 illustrates the structure of the HVAC system used for room conditioning. Heating is provided by two sources: a solar thermal system and a heat pump operated with ground water. Cooling is provided directly from the ground water. The heat is injected into the room via four lines of thermally activated building systems (concrete cores), each of which supplies the cores in all floors of each quadrant (NW, NE, SW, SE). The installed state of the art room temperature control generates set points for the desired TABS temperature for each floor and each zone as a function of the current ambient temperature. Furthermore, a desiccant cooling system, regenerated by heat from the solar thermal system, supplies cooling power for the air conditioning system.

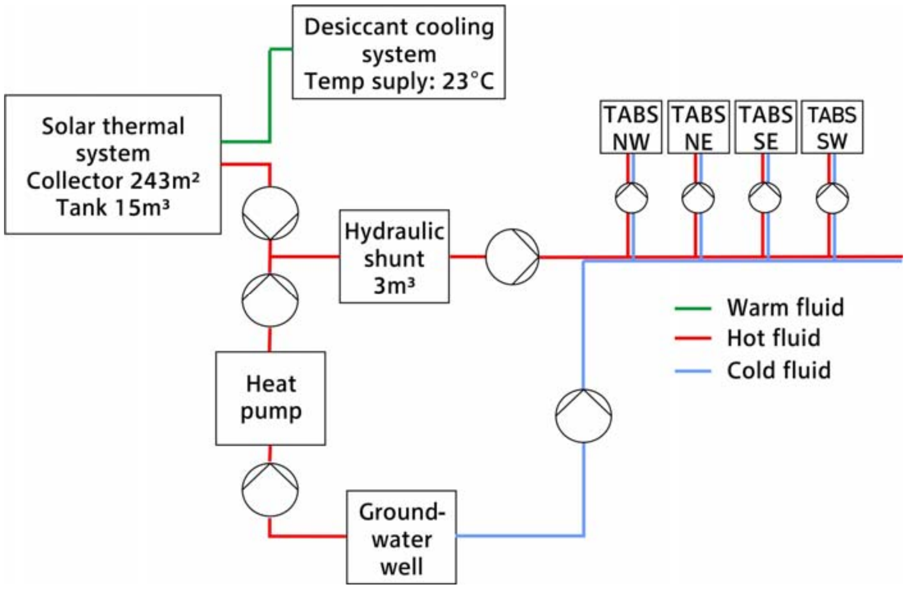

Figure 53: Overview of heating and cooling system Energy Base

Since the building was already subject to previous research projects all the information about the system design, sizing and control algorithms was already known and only had to be collected, organized and distributed among the project partners.

Intended uses and use case

The intended use was already determined to a large extent by the proposal. It is, as mentioned before, to test a model predictive control solution in the first step by simulating the reaction of the building and in the second step to integrate the MPC into the real-building. The second step in this process signifies that the intended use is a real-time application with a HIL component.

Since the purpose of this modeling and simulation project were two unique applications only two use cases existed in this particular case: the HIL application and the test simulation. Since the test simulation is a simplified version of the HIL application, more thought was put into defining this use case. Therefore, in this phase of the project a lot of work was put into the detailed identification of the load shift potentials and the specification of the interfaces, where the MPC could influence the building.

Considering that the storage potentials, that seemed promising to present load shift potentials, were thermal and the demand that should be shifted was electrical, the obvious implication was that the components connecting those two systems had to be targeted: the heat pump and the ground water well pumps. Both represent relatively large electricity consumers and using the relatively inert system of the TABS the electrical loads for heat and cold production from the well could be shifted to convenient time slots.

With regards to the implementation of the interfaces of the MPC and the current building control system the only feasible point to influence the installed control system was to modify the set-points for the ceiling temperature levels and the set-point temperature of the water in the supply line to the concrete cores. Another important aspect of the use case is that prediction of the system behavior at a certain point in time must rely on a prediction of influences on the system, which have to be provided and integrated into the simulation.

The test simulation use case differs just so far that the real building was substituted by a model of it and the prediction data was substituted by historical data.

Requirements

From the objectives, the system description, the intended uses and the use case the requirements for the simulation were defined for the HIL application, which were in a reduced form applicable for the test run as well.

Functional requirements:

- The MPC algorithm must be part of the simulation.
- The MPC algorithm must produce modified set-point temperatures as an output.
- A thermal building model, which receives the set-point temperatures from the MPC algorithm, must depict the whole control process from set-points to comfort conditions in the rooms and electric energy demand.
- All outer and inner influences (disturbances) on the energy demand of the building must be predicted and the prediction must be kept up-to-date and integrated in the simulation.
- A second model for the control path must exist in order to substitute the building in the test simulation.
- An interface to link the simulation with the building automation system must be implemented.

Concerning the non-functional requirements, the application in a controller raises some additional challenges. Mainly the simulation (control algorithm and model) must be fast enough to match the real-time requirement. Another important requirement is added numerical stability in order to avoid crashes during controller operation. This concerns initialization as well as numerical execution. Furthermore, integration with the building automation system must be possible.

6.3. Conceptual Model and Design Model

Based on the requirement definition the conceptual model was derived. Subsequently the conceptual model on building level is described into more detail and the connection to the grid model is briefly addressed for sake of completeness.

Figure 54 shows a graphical overview of the conceptual model for the building level MPC integration and test simulation. The model structure is again based on the general description of the components and the variable connections, described in Chapter 3.3, representing the influences of the components on each other and each model component represents a defined part of the overall system and can in any case be presented in a single modeling environment. Special attention was paid to the interchangeability of certain parts of the simulation against real existing systems, in order to be able to build both, the test simulation and the HIL application, on the generic model.

In the conceptual model green ovals represent the system building and facilities, as well as the external influences. As part of the test simulations this part is represented by a complex model and historical data for weather and users influences in the building. As part of the HIL run this part of the model is replaced by the real building. The blue ovals represent the elements of the model predictive controller. The controller (MPCB – model) essentially consists of the prediction data for the user behavior and the weather, a simplified model of the building and the building services (SBUI and SBS), and the MPC algorithm (MPCB). The components illustrated by dots are external factors that cannot be influenced by the system (disturbances of the control). Subsequently a short overview of the components of the model will be given.

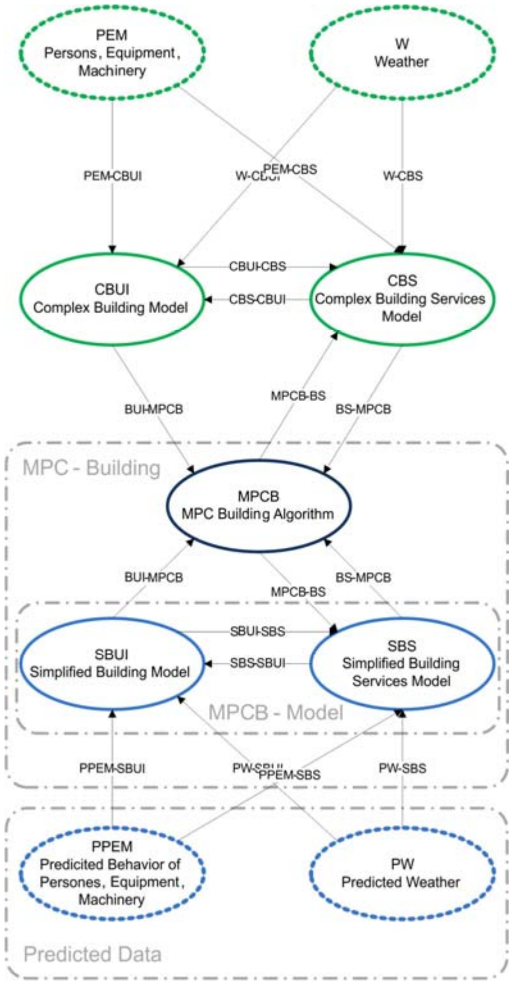

Figure 54: Conceptual model for the building MPC model

PEM – Persons, Equipment, Machinery

PEM describes the behavior and physical impact of the humans and the equipment they operate within the building as far as it influences the buildings behavior (e.g. waste heat, electricity demand...). In simplification it is assumed that this behavior is not influenced by the state of the system (i.e., no additional feedback such as people leave a building due to unsatisfying thermal comfort).

W – Weather

The component W represents the weather around the building as far as it influences the buildings behavior or the building services.

CBS – Complex Building Service Model

CBS describes the whole building energy system. Conversion, distribution and storage within HVAC systems, other thermal systems and electric systems are modeled within this component. Control strategies not accessible to the MPC are modeled in this component.

CBUI – Complex Building Model

CBUI contains a thermal building model. Also simple controls of building parts as long as they are not accessible to the MPC are modeled within this component. This includes mainly controls of systems that affect the thermal state of the building but have a control that is not mainly governed by thermal aspects (e.g. controls for moveable shading devices). Core activation is modeled within this component not CBS, due to technical reasons. The water provided for the activation is supplied by CBS.

MPCB – MPC Building Algorithm

MPCB models the control algorithm used by the MPC that controls the building. The models of the system influenced by the MPC algorithm are not contained in this component; they are subject to SBUI, SBS. Furthermore, the models to depict the disturbances inflicted upon the system are not included in this component either. They are depicted in PPEM and PW.

SBS – Simplified Building Services Model

SBS is the simplified model of CBS implemented within the MPC. It encompasses physical components of the building services and control strategies not accessible to the MPC. SBUI and SBS together represent the controlled system.

SBUI – Simplified Building Model

SBUI is the counterpart of CBUI implemented within the MPC. SBUI and SBS together represent the controlled process.

PPEM - Predicted Behavior of Persons, Equipment, Machinery

PPEM is the model of the prediction of persons, equipment and machinery provided for the MPC. PPEM is considered a disturbance for the MPC. Due to lack of reliable prediction models for the user behavior PPEM was substituted by historical data for comparable time periods (time of the year, weekday).

PW – Predicted Weather

PW is the model of the prediction of W provided for the MPC. PW is considered a disturbance for the MPC. The weather prediction was supplied by the Austrian meteorological service and uploaded to the simulation framework on a daily basis.

To conclude the conceptual modeling process of the simulation at building level, a documentation of the components in template form, similar to INFO, was complied.

In order to provide a context to the grid simulation Figure 55 provides an overview of the conceptual model of the two main focal points of the simulation the building and the network, which are simulated independently in order to facilitate the technical implementation of the simulation. This approach does not take into account the interaction of the two systems. Therefore, restrictions inflicted by the two systems upon each other, are considered in the design of the MPC. However, this approach creates the necessity to duplicate parts of the building model, because the simulation scenario to be tested assumed several MPC controlled buildings would be connected to the grid. Therefore, simplified copies of the building MPC model were integrated into the grid MPC in order to represent the interaction between the two

MPCs. The consumption behavior of buildings equipped with a building MPC was represented by simplified copies of the whole building simulation.

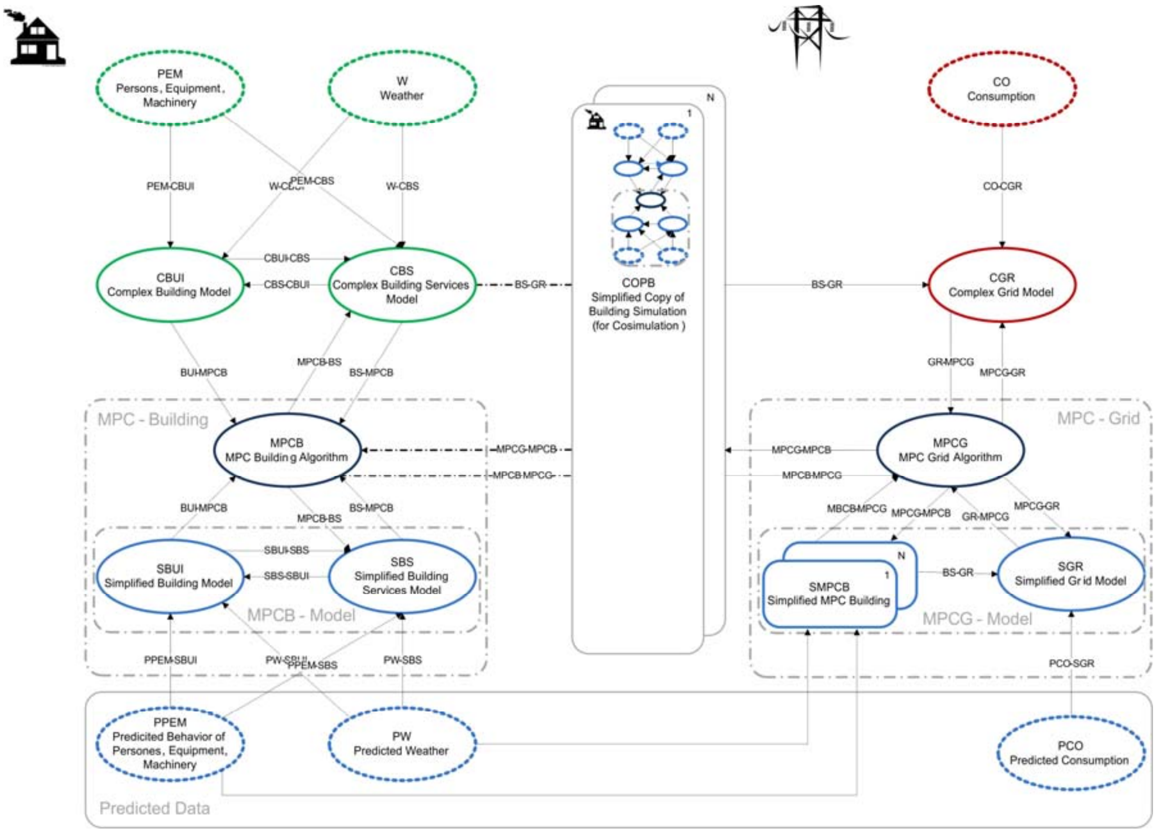

Figure 55: Conceptual model of the simulation of the building and grid

In the next step of the modeling process the conceptual model was developed into a simulation model. As mentioned in Chapter 6.1 three M&S groups were engaged with the building modeling process. The building expert group 1 had access to all data resources concerning the building. Therefore, it was decided, that they would develop the complex building model and building service model which was to substitute for the building in the test simulation. Based on the complex model, the second building expert group, to which the author belonged, would derive a simplified model to be deployed in the MPC. The control theory experts were of course concerned with the MPC algorithm development. Both building experts preferred Dymola as a simulation tool, the control theory group worked in Matlab. The final simulation model can be seen in Figure 56. The topmost oval of the simulation model represents the complex building model in the test simulation and the real building for the HIL application. Furthermore, in the test simulation the yellow oval at the bottom could be integrated into the simplified system simulation as well, since historical weather data was used, which could be implemented as a simple lookup table.

Concerning implementation of the test simulation a co-simulation approach using Matlab as a master was chosen. In the HIL application matters are a little more complex. Matlab still is the simulation master initializing simulation runs of the simplified Dymola model when needed. After completion of the simulation run, the results, which consist of trajectories of certain state and process variables calculated by the simulation in Dymola are returned to Matlab. The interface with the predicted weather stays the same from the Dymola point of view, but the lookup table is periodically updated. To implement the interface between simulation and the real building the automation solutions provider developed an interface that ensured the data exchange between Matlab and the building automation system.

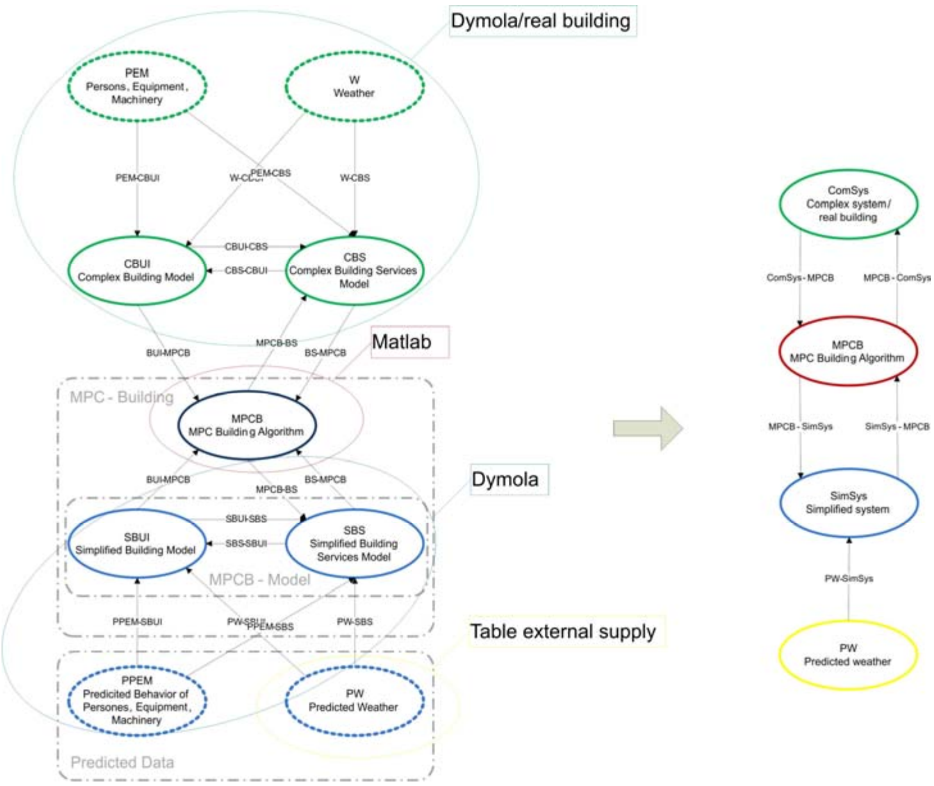

Figure 56: Reduction from conceptual model of Building MPC to simulation model

Apart from the technical implementation also the temporal management between the components of the simulation and building is more complex. The MPC needs its model to simulate ahead in order to have information about the behavior (trajectories) of certain system variables over the whole prediction horizon. Therefore, the co-simulation must be executed in a sequential manner and the temporal sequence depicted in Figure 57 results.

First the interface of the building automation system with Matlab transfers sensor data of the real building at time t to Matlab. This data consists of important system temperatures, needed as a feedback for the controller or to initialize the model. Since the sensor data does not correspond entirely with the calculated state variables in the simplified building model in terms of spatial granularity, a mapping process is carried out in Matlab. After this step Matlab transfers the temperatures at time t to Dymola. These temperatures are required to initialize the Dymola model, because if the simulation starts with incorrect initial conditions of the dynamic storage components, especially the concrete cores, which have time constants of days, a huge error would be produced. Furthermore, the set-point temperature trajectories for the prediction horizon and the start time t are communicated to Dymola. Using the start time, Dymola reads the predicted data for the disturbances from the look-up tables and calculates the system behavior based on the set-point temperatures supplied by the MPC for the prediction horizon, which is in this case 48 hours. After terminating the simulation the trajectories over the prediction horizon of certain state variables (mainly TABS and room temperatures) and energy flows are reported back to Matlab, where the MPC algorithm starts to calculate the new set-point temperatures for time $t + 1$ and the trajectories for the next 48 hours beginning with $t + 1$ that are needed for the next building model simulation iteration. After supplying the new set-point temperature to the building the cycle is terminated and starts from the beginning. It must of course be taken into consideration that the calculation time for one cycle must be shorter than the set-point modification interval, which was in this case chosen as 15 minutes. Otherwise the simulation would fall behind the real system and would fail its purpose.

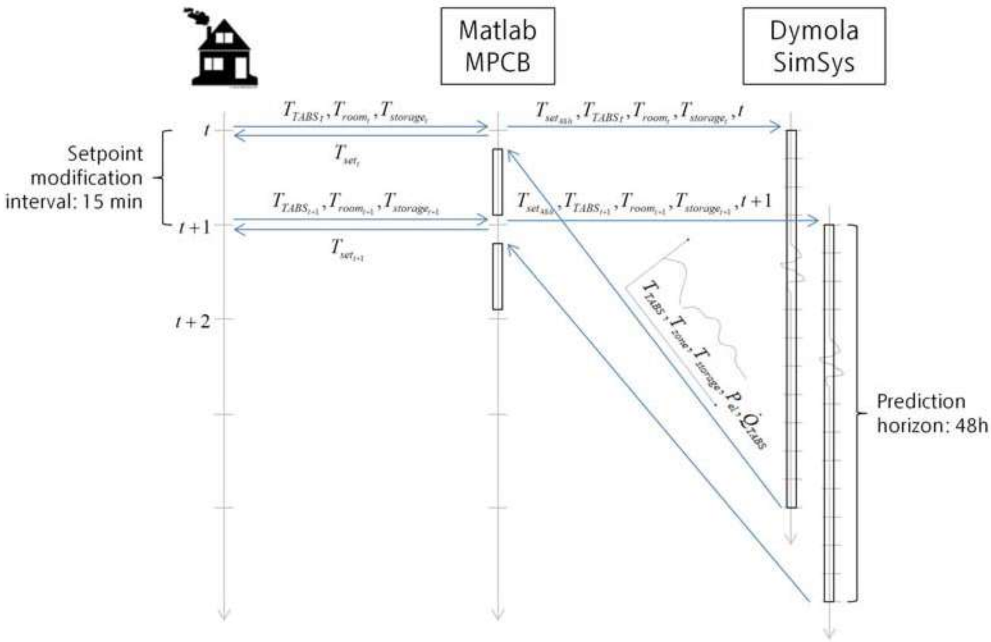

Figure 57: Temporal sequence of CoOpt HIL-simulation

6.4. Sub-Model Energy System

As mentioned above the building expert group 1 had access to all data resources concerning the building. Therefore, it was decided, that they would develop the complex model based on which the second building expert group, to which the author belonged, would derive a simplified model to be deployed in the MPC.

The complex building model was based on the "Beuken-model" approach [150] which represents the building's thermal zones by RC-networks. This modeling approach is a good compromise between model simplification and model quality. The model is described in more detail in [151]. Furthermore, the heating and cooling system was modeled using Modelica's acausal thermal and hydraulic library. However, the model still showed a degree of complexity that could prove troublesome for application in an online optimization problem. Therefore, in order to further simplify the model and increase stability and computing speed, a few more simplifications were applied. Special consideration in the process was given to calculation speed and stable performance in order to meet the requirements resulting from the intended use.

The choice of modeling standard and simulation environment again fell on Dymola/Modelica, because of the interoperability, the already existing expert knowledge and model libraries from previous projects, which were used to model the building services. Besides choosing the modeling environment, several measures of model reduction were applied to the complex building model in order to obtain a sufficiently compact model for use in an online optimization problem. The signal flow based approach described in Chapter 4.1 was chosen instead of the acausal modeling approach Modelica suggests. As mentioned when introducing this approach, it eliminates the need for calculation of the state variables of the fluid at each relevant point of the hydraulic network, but opens up new problems, as the state variables at these points, mainly the temperatures, are used as a control variables. This was especially critical in this case because the control path leading from the set-point temperatures to heat injection into the TABS had to be modeled accurately in order to fulfill the model requirements. Therefore, alternative approaches had to be developed to approximate the control strategies of the system. These are mainly based on temperatures of thermal storage masses (e.g. storage tank, concrete core) in the system.

In order to achieve a simplification of the building model, the thermal zones of the building were united into larger substitutional zones. In this process, the areas supplied by a line of the concrete core, were combined into one zone per floor. The building has 4 lines, which supply the 4 quadrants of the building (NW, NE, SE, SW). With this measure, the number of thermal zones of the building model was reduced from 66 to 18 zones. This approach could be chosen because the temperature profiles of the active zones in the individual quadrants deviated only slightly from each other.

Furthermore, for the models of thermal R-C components, the graph-connected components were substituted by simplified models, which are based on energy balances and equations describing the heat transfer resistances. Despite using fundamentally the same physical description, this approach reduced the number of equations significantly - from 94 to 24 in case of an active thermal building zone model. The modeling approach is described in more detail in Chapter 4.4.2. In order to map the measurement of the 66 building zones to the 18 values of the simplified model at the model interfaces, temperature averages weighed by heat storage capacity were used.

By applying the described model reductions the number of non-trivial model equations was reduced from 24453 in the complex model to 1080 equations. The simulation time shortens correspondingly. For a the simulated time of 48 hours, which corresponds to the prediction horizon, with a time step of 15 minutes, running on a standard PC, the computing time for the simplified model is about 1 second while the complex model required 175 seconds. This delivers some proof that the model abstractions introduced in Chapter 4.1, actually offer considerable advantage in terms of system complexity in comparison to physical and acausal modeling paradigms.

From applying these model reductions, a simplified model architecture as shown in Figure 58 results. The simplified building and energy system model is made up of three main components that represent the total control loop installed in the building: the model of the building with 18 thermal zones, the model of the heating and cooling system, and the control, as it is active in the building.

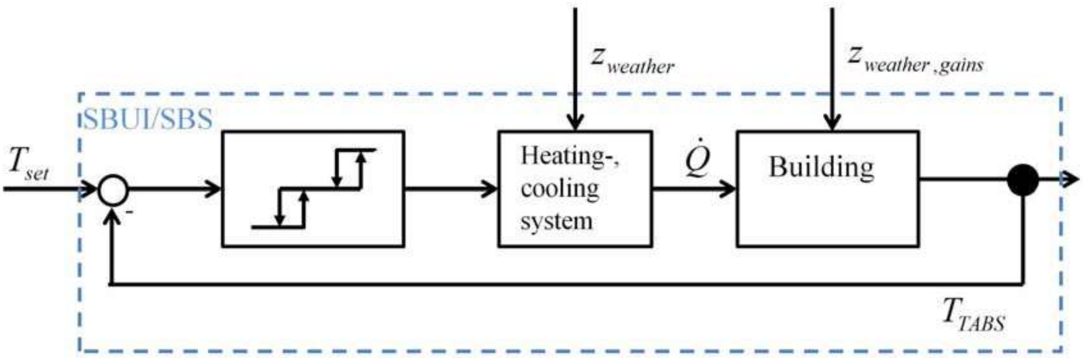

Figure 58: Block-diagram of the simplified building model

The controller receives set-point temperatures from the model predictive controller for each concrete core, as well as for the supply temperature to the lines as a command variable. For these set-point temperatures, the model of control assesses the heat flows to be delivered to the concrete cores, out of which the model of the heating and cooling system calculates the demand for electrical energy.

The heat flows are transferred as manipulated variable to the building model, which provides the thermal state of the rooms, concrete cores and thermal storages as feedback to the model-internal control, as well as to the model predictive control. Furthermore, the MPC receives heat flows into the TABS and electric power consumption as input-information from the model, although there is no real-world sensor capturing this data. The weather acts as a disturbance for the heating and cooling system and the building. Another disturbance, that affects only the building, is represented by the users and the influence of the ventilation system. The described heating and cooling system includes the determining components for the heating and cooling of the building: The well pump, the heat pump, the hydraulic joint, the solar storage tank and the solar thermal collector. Figure 59 shows the Dymola model resulting from this structure.

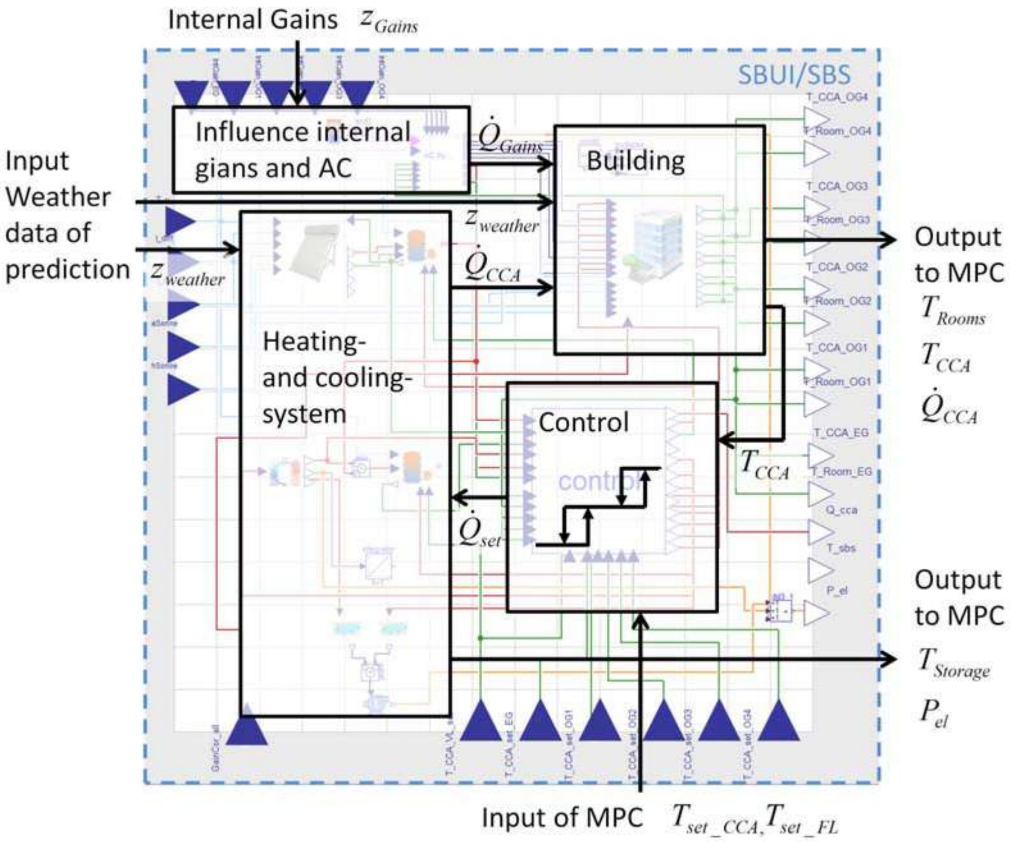

Figure 59: Model architecture of the simplified model in Dymola

6.5. Validation and Verification

Contrary to the model assembled in INFO the model of this project could be validated by comparing the simulation results to real world data and also by comparing the complex and simplified model to each other. Apart from comparing results several validation and verification sessions during which the modeling team of the complex and simplified model thoroughly checked the model of the other team. Several such verification and validation sessions were held during the development process of the models at different stages of model evolution.

Furthermore, the component models were of course verified and validated according to the principles described is Chapter 4.2. The control model of the simplified model was also equipped with several assertion checks, in order to ensure the workarounds applied to make up for the lack of state variables were valid.

The comparison of the results was carried out in two steps. First the complex model results were compared by the developer to monitoring results of the real building. The result of the comparison of the room temperature of a certain zone can be seen in Figure 60. The modeler concluded that the deviation of the temperatures towards the end of the simulation time is due to simplifications in boundary conditions to the adjacent zones and floors [151]. It must however be noted that a similar deviation of room temperatures occurred between the simplified model and the real building during the HIL application and that it had to be solved by applying corrective heat flows to the model.

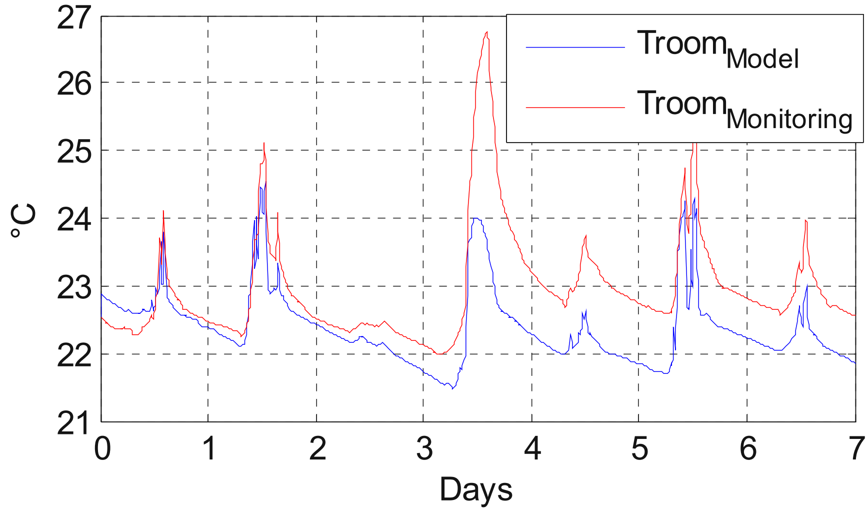

Figure 60: Validation results for the room temperature of a reference zone [151]

In the next step the complex and the simplified model were compared in terms of calculated electric energy demand and room temperatures. Figure 61 shows a comparison of the calculated electric energy demand of the heat pumps, which constitute a major part of the load shifting potential over a period of two days in January. Figure 62 compares the temperature profiles of three thermal zones in the southeast quadrant of the building simulated with the complex model to the temperature of the substitutional zone of the simplified model during the same time period. Zone 1 and 3 in the complex model are actively influenced by the TBAS and have a significantly larger thermal mass then zone 2, which is a staircase attached to the outside wall and not heated or cooled by the TABS. Therefore the temperature profiles differ. But the simplified model shows very good accordance with the behavior of the two larger zones, which are determining for the thermal behavior of the sector. Overall the accordance between the two models appeared to be satisfying for its intended purpose.

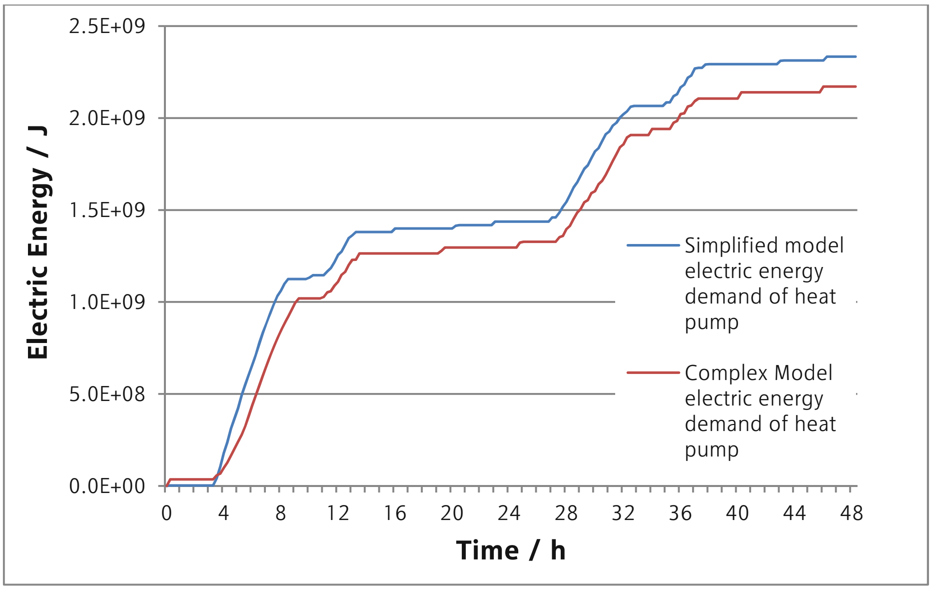

Figure 61: Cumulated electric energy demand of heat pumps comparison between complex and simplified model

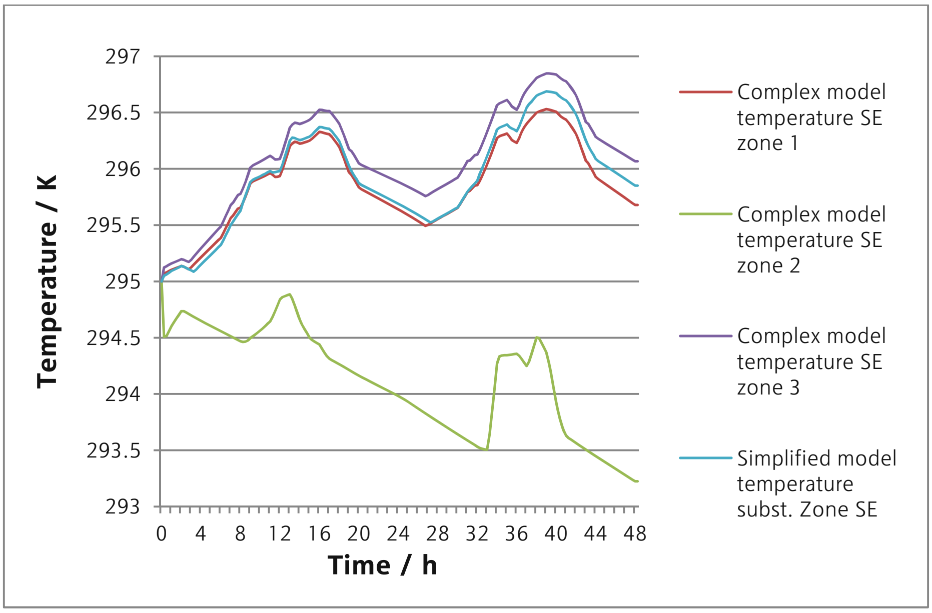

Figure 62: Temperatures in thermal zones comparison between complex and simplified model

6.6. Implementation and Results

In order to estimate the potentials of the load shift a comparison between results without and with model predictive controller was performed using the test simulation setting with the complex building model instead of the building. As a baseline scenario the conventional control scenario was simulated and then compared to a scenario with active model predictive control. Figure 63 and Figure 64 show the result for two winter days simulated with historical weather data. According to the simulation the optimization potential is significant. The electric energy consumption of the pumps could be reduced to 30% of the original amount. The simulation study was carried out by the control theory group and contributed to a joint publication [151].

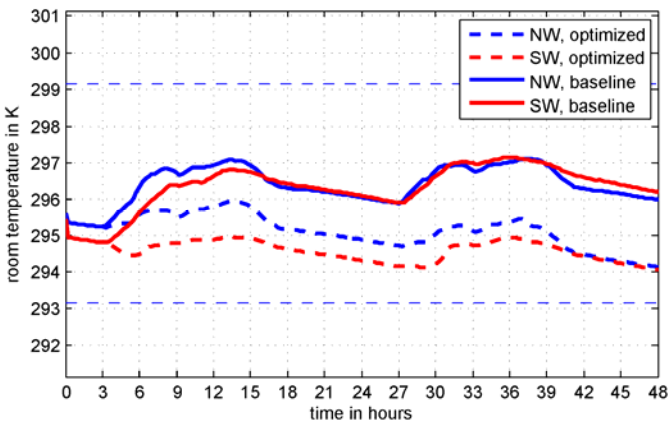

Figure 63: Selected room temperatures evaluated in the defined load shifting scenarios (2 winter days) [151]

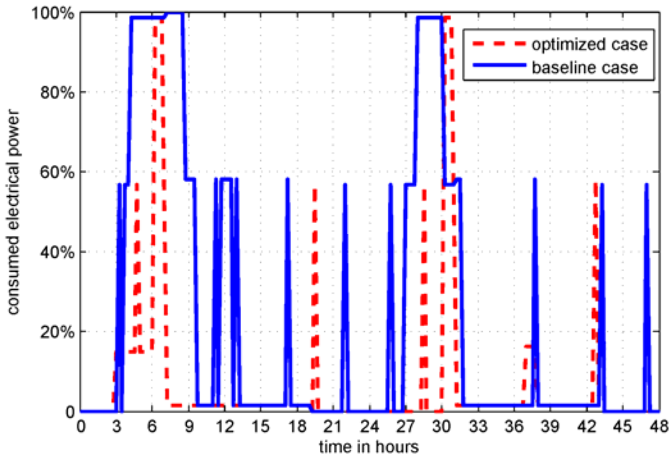

Figure 64: Total electrical power consumed in the defined load shifting scenarios (2 winter days) [151]

Concerning the results of the application in the real building it could be confirmed from the monitoring data, that the MPC was active and working, however it has not been in action long enough to make any resilient statement concerning the saving potentials. At least it could be proven that the application of M&S applications in complex real-time control applications is possible and that by application of these techniques load shifting actions to realize effective demand side management for buildings can be implemented.

7. Process Modification for Balanced Manufacturing

As addressed in the previous chapters the manufacturing industry is one of societies' largest energy consumers and promises major reduction potentials. Concurrent increase of legislative pressure and progressive resource shortage have caused manufacturing companies to streamline their production in order to increase the efficiency of resource usage, especially targeting energy consumption and CO_2 emissions. Triggered by this demand, a variety of methods and separate tools for improvement of single aspects of energy efficiency within production facilities have already been developed, such as energy efficient machinery, optimization of stand-by-modes, use of waste heat, improvement of building hulls, use of renewable technologies, life cycle analysis and sustainable products design (also see Chapter 5.1). The research presented in Chapter 5 contributes to this area of research as well, by developing an integrated planning tool for production facilities.

However, since the beginning of the INFO project research has proceeded and new questions have arisen. As previously mentioned, efforts in the direction of energy efficiency are inhibited by a number of factors, the most determining among them are long payback periods, lack of ownership and supportive tools [136], [138], [139].

A gap analysis of existing research and industrial needs [137] identified two main development demands in order to enable efficient and effective energy management: production management with regard to energy efficiency and integration of energy efficiency performance criteria into information and communication technology (ICT) systems. Available solutions for measurement, control and improvement of manufacturing processes are not generally suitable for energy management in production companies, neither on the plant level nor on the process level. The gap is seen in the actual implementation in industrial companies. From the technological point of view [138] sees major benefits in simulation techniques that predict energy and resource flows for large manufacturing systems, particularly highlighting the simulation supported optimization of production planning.

Another interesting aspect is the fact that industry can be seen as a major opportunity to balance the electrical energy market by demand side management of large-scale industrial enterprises. [152] estimates that demand side management stemming from large-scale industrial plants could be able to provide approximately 50% of capacity reserves for the positive tertiary balancing market in 2020. Therefore, solutions to integrate the industry into smart grids must be developed.

In order to address these challenges, methods to integrate energy related data into ICT systems, such as [153], [154] and numerous approaches for systematic energy efficiency improvements, e.g. [143], [155]–[158], have been developed. Concerning simulation applications for manufacturing, methods for analyzing singular aspects of the system ([159]–[161]) as well as comprehensive planning tools ([162], [163] and the previously described INFO tool) have been introduced. However, these tools are targeting analysis and planning, exclusively. A systematic, comprehensive approach for assessment and optimization of energy- and resource-flows during operation of production facilities is still deeply lacking.

Hand in hand with the integration of energy performance measures in ICT goes the research question of suitable key performance indicators (KPIs). Carbon Footprint of Products (CFP) are a commonly used benchmark to identify the environmental impact of products. CFPs are usually assessed on a one-year-basis. They are considered an important instrument for raising awareness on the customer sides, as well as within the company. Raising awareness is an important step towards energy efficiency, since research showed that awareness, especially of the management, is one of the factors significantly affecting the CFP in companies [164]. However, surveys of currently available standardizations and tools have brought up some issues with the reliability of results due to incomparability of different methods and lack of reliable data [133], [165], [166].

The usual top-down approaches for calculating footprints are even less suited to support sustainable plant operation, because they lack the temporal and spatial resolution necessary to base resilient statements upon them. [167] concludes, that one aggregated indicator is essential for communication but failing to provide the required detail to undertake a meaningful assessment. Footprints need to include both aggregated and decomposed figures, because while the static aggregate may remain roughly the same over time, the contributions to it may change significantly. Katharina Bunse hits the same line by demanding energy efficiency metrics on plant and process level and stresses the industry's need for real-time data and knowledge-embedded processes leading to significant KPIs (key performance indicators) of energy efficiency [137]. A CFP of adequate temporal and spatial resolution could serve this purpose as well as be a means of communication to stakeholders. Some research has been attributed to extending CFP methodologies into this direction. [168] meets this demand by providing a methodology for assessing a time-resolved footprint of the supplied energy. [169] attempts to integrate a higher resolution into product footprints by means of simulation. In order to address these issues comprehensively, a bottom-up approach for aggregating a product footprint incorporating the whole production phase of the product life-cycle is needed.

7.1. Objectives of Balanced Manufacturing

Therefore, the idea of Balanced Manufacturing was developed. Most generally speaking, Balanced Manufacturing, short BaMa, tries to couple sustainability with competitiveness in industrial production, by finding a balance between energy and cost efficiency. It is a methodology for monitoring, predicting and optimizing the energy and resource demands of manufacturing companies under consideration of the success factors time, costs and quality. Based on the methodology, a software tool chain will integrate the Balanced Manufacturing methodology into industrial automation systems, in order to assist energy conscious steering of a plant during operation.

Two aspects set BaMa apart from the other energy management systems and optimization tools discussed above. First is its comprehensive approach. Although a variety of methods and tools for increasing energy efficiency exist, the majority focuses on singular aspects of energy efficiency or application areas. BaMa takes more than one application field into account, when analyzing the system for optimization potentials. It addresses the production, the building, the energy system and the logistics.

Moreover, BaMa is not a design or analysis tool, which focuses mainly on assessing existing systems or finding improvement potentials in the design of a production or the supporting infrastructure. BaMa is a planning tool that assists in operating a production facility in a balanced, energy efficient way, much like an advanced planning and scheduling system would support a cost and/or time efficient production process. [170] identified four classes of attributes, which determine the objectives and criteria for decision making in manufacturing: cost, time, quality and flexibility. These criteria are usually the planning targets of common scheduling tools (such as Simio, Lean Factory Management, Siemens PLM, etc). Balanced Manufacturing adds another factor, taking the environmental impact into account, into the equation. So, in a nutshell, BaMa introduces energy as a steering variable into the plant's operational planning.

In order to meet the discussed challenges and integrate all the desired functionality the BaMa tool chain contains three core modules:

- Monitoring: Data on resource consumption are aggregated and visualized. Monitoring results serve as a reporting document and help to identify technical and infrastructural optimization potentials. This makes BaMa compatible with the requirements of the energy management standard ISO 50001, which is based on the Deming Circle or Plan-Do-Check-Act principle and therefore demands for a mechanism to assess the targeted results.
- Prediction: Based on data and numerical simulation-models of machines, equipment and infrastructure, this part of the tool chain allows forecasting of the overall energy demand of the plant based on the production plan and other forecasting data (e.g. weather information). This feature is especially useful for day-ahead planning of energy demand and production and can therefore aid with demand side management and the integration into smart grids.
- Optimization: Based on the results of repeated simulations, an optimization algorithm improves the plant operation with regard to the optimization targets energy, time, costs and restrictions such as resource availability and quality. The optimization targets especially towards minimizing energy demand by using synergies, peak load management and optimized use of available equipment.

Using monitoring data and simulation results, BaMa can derive an individual dynamic product footprint for single products or batches. The product footprint represents a product's expenditures concerning cost, time, energy and the environmental impact such as resulting carbon emissions in the product life cycle phase within the factory (gate-to-gate).

As mentioned above, BaMa is a tool that is designed to support the operation of a production facility in a balanced, energy efficient way. Therefore, BaMa is ideally utilized periodically during the operation of the plant in order to compute optimized strategies for the plant operation. To ensure the tool chain's functionality in this respect, it will generally have to be embedded into the automation systems of the company. There are a variety of challenges that can be addressed with the help of BaMa. Figure 65 gives an overview of conceivable use cases for the application fields and the different modules of BaMa in the four fields of action.

	Machines and production process	Building	Energy system - TBS	Logistics	Overall Application
Monitoring	• Monitoring of energy demand of certain production processes or steps • Condition monitoring via energy data analysis	• Monitoring of room conditions in order to avoid violations of comfort conditions	• Monitoring of energy flows within company • Monitoring of energy converters and storage charging level • Error detection	• Monitoring of energy demand of transport processes and storage • Condition monitoring of transport systems	• Comprehensive energy monitoring and reporting tool according to ISO 50001 • Calculation of gate-to-gate product footprint
Prediction	• Prediction of production energy demand based on production plan	• Prediction of heating and cooling energy demand based on weather data and production schedule	• Prediction of demand of different forms of energy based on demands of production, logistics and building	• Prediction of energy demand for transport and storage based on production schedule	• Prediction of total final energy demand • Intelligent connection to smart grids
Optimization	• Peak load management • Scheduling of tasks achieving minimized labor and energy costs	• Optimization of heating or cooling schedules according to production plan and weather	• Optimized operation strategies for available equipment • Optimized use of storage potentials	• Minimization of covered distance of means of transport • Energy or cost optimized timing of transport activities	• Global energy or cost optimum considering degrees of freedom in all action fields

Figure 65: Use cases for BaMa according to modules and optimization fields

Although BaMa can address many challenges faced with, when dealing with energy efficiency, it also has limitations. Due to its nature as a planning tool, that is supposed to support the daily operation of a plant, there are some functionalities that BaMa does not provide: It is not a tool for optimization of technology or design, but focuses singularly on the interaction of system components. Concerning the footprint, only the part within the factory is taken into account, not the whole life-cycle of the product. Other crucial points BaMa needs in order to operate successfully are degrees of freedom and a data base. Optimization is impossible without degrees of freedom. On the other hand if the number of degrees of freedom becomes too large, computation time or required processing power will grow beyond a feasible point. BaMa cannot perform an optimization without data about energy, costs or availability of resources. This data will have to be collected from monitoring, measurements or other automation systems.

7.2. Methodology for Conceptual Modeling for Balanced Manufacturing

As mentioned in the previous section the outcome of Balanced Manufacturing is a simulation based tool-chain. Therefore, the model of the simulation is one of the core parts of the tool-chain and the structure must be well-considered because its application poses some additional challenges.

Primarily, it needs to be taken into consideration that although the tool chain may be an almost entirely reusable software solution, the model within the software tool-chain represents a unique plant. Therefore, it must be assembled for every specific instance from scratch, which means that the software development and integration process must be extended to a second layer. A modeling process accompanying every single implementation must be added. Figure 66 illustrates this concept based on a software-lifecycle, given in [36, p. 13].

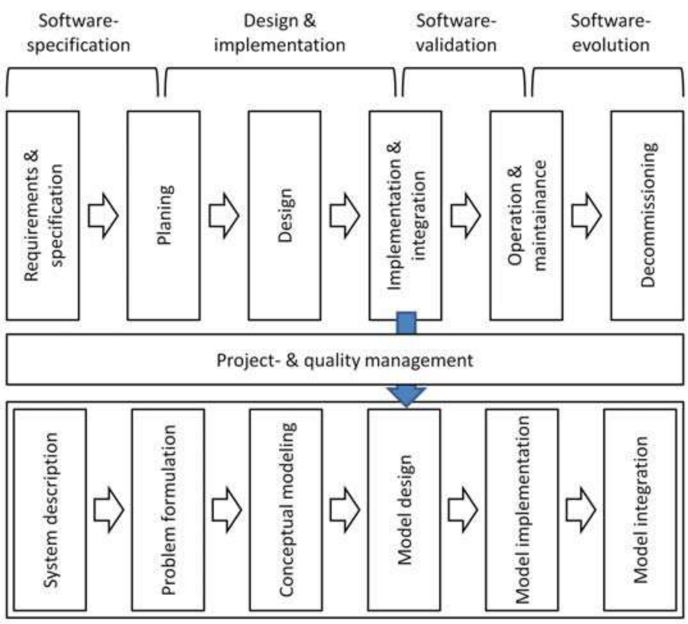

Figure 66: Extended Software Life-Cycle

The modeling process represents a considerable effort, which can only be reduced if a certain degree of model reusability can be achieved. A number of researchers concerned with medium to large scale simulation models have suggested decomposition or modularization approaches at model design level, to ensure model reusability [28], [53], [54]. Similar design principles are recommended in object oriented software engineering, where apart from modularization and decomposition also encapsulation and information hiding play an important role. Encapsulation aims at hiding internal details towards the external and only providing necessary functionalities and properties. Communication usually takes place via interfaces. As long as the interfaces remain unchanged encapsulated system parts can be exchanged without affecting the overall system behavior [36, p. 29]. This suggests that the decomposition approach described in the previous chapters could be developed into an efficient framework for Balanced Manufacturing, if the interface definition could be elevated to a more generic level and standardized.

The developed Balanced Manufacturing methodology is the basis for the tool chain and represents the core concept of BaMa. It has two main purposes i) to serve as a guiding principle for analyzing a manufacturing system prior to the implementation of BaMa, and ii) to serve as a concept for the development of models of the production facilities, which are needed for the simulation the tool chain is based upon. The chosen methodological approach is designed to address the high system complexity and heterogeneity by dividing the overall system from an energetic point of view into well-defined manageable modules, which then allow a focused system analysis independent form the surrounding environment. The methodology BaMa follows is formulated at a very generic level to ensure its usability in a variety of production facilities and the reusability of components.

The basic module of the system analysis is called “cube”. Cubes have a clearly defined interface and represent a certain physical behavior that contributes to the resource balance of the overall system. In other words: cubes are balances. This approach, inspired by common approaches from fluid mechanics or thermodynamics, was chosen over the usual process approach, because it corresponds more intuitively with the object-oriented paradigm of modularization. Cube boundaries bundle balances in terms of energy-, material-, cost- and information flows in the same physical place and therefore decompose the whole system into observable parts. Cube boundaries are of course imaginary. However, in most cases they will coincide with some sort of physical representation. A cube can be for instance a machine tool, a chiller, a baking oven, the production hall or a utility system. In a BaMa monitoring system, sensors would preferably be installed to measure flows at cube interfaces. Figure 67 illustrates the concept of cubes.

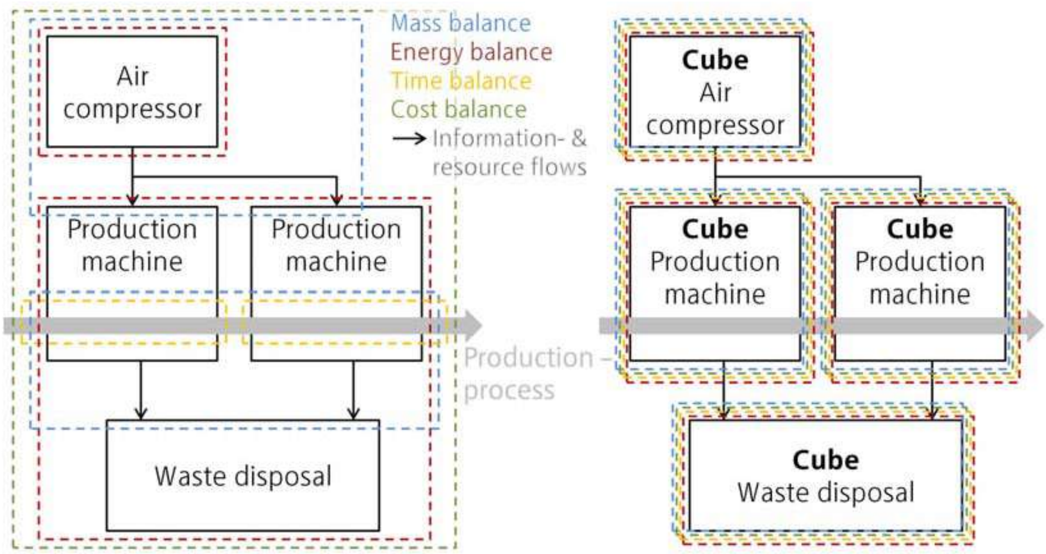

Figure 67: Concept of cube decomposition

The cube approach offers a variety of advantages, not only from the perspective of system analysis, but also from perspectives of knowledge management, model design and technical implementation. The cubes are also the building blocks of the model, i.e. the prediction of the behavior of the plant assuming certain scenarios results from a dynamic simulation. The results of the simulation form the target function for the optimization algorithm. So, the prediction and optimization use models of the cubes (virtual twins of the real cubes) in order to simulate the behavior of the system parts. Figure 68 shows the relationship between real and virtual cubes in the simulation environment and the integration into the overall automation system architecture. On the lower right, the real system with the imaginary cube boundaries is shown. The real system interacts with the plant's automation system via interfaces. Sensors measure data and actors apply control actions. The automation system routes data between the BaMa tools and the real system, supplies additional data e.g. from enterprise resource planning or manufacturing execution systems and integrates BaMa into to control centre. With this approach, the cube methodology exactly translates the recommendation of decomposition and modularization. The modular system architecture offers flexibility and reusability of model parts.

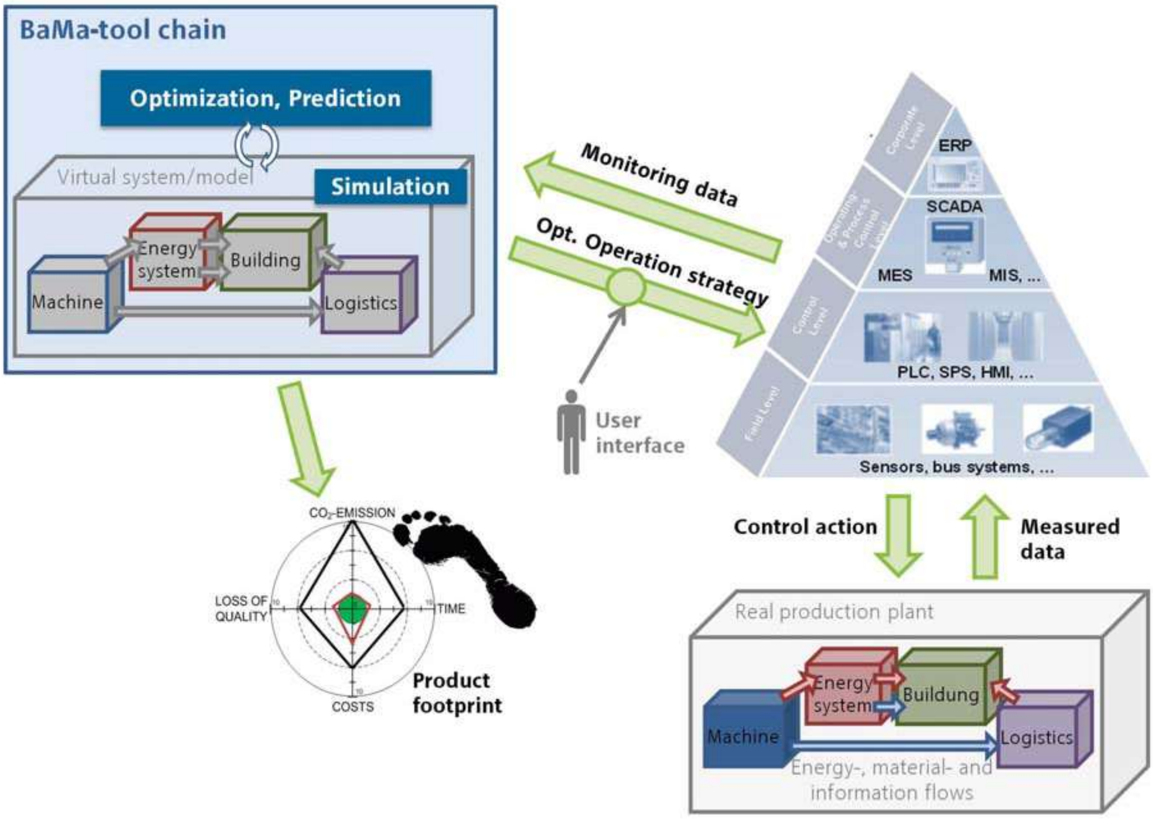

Figure 68: Architecture of BaMa tool chain

As mentioned above, cubes unite system boundaries concerning energy-, material-, cost- and information flows, which enable the specification of the concept of a cube in its most generic form by simply specifying its boundaries, which are in terms of the model represented as interfaces. Specifying the interfaces of cubes generically in a way that every model of physical objects related to energy balances in production plants can be housed within them offers two main advantages. The boundary specification enables encapsulation and information hiding and therefore coupling of different modeling approaches and degrees of model abstraction. Furthermore, the generic description of cube attributes and interface definition guaranties the applicability and compatibility of simulation models for all parts of the plant and for different kinds of productions.

Figure 69 gives an overview of the interfaces of a generic cube. Information flow provides operating states and monitoring values for the higher level control as well as control actions for the cube module. All necessary energy flows (electrical, thermal, etc.) are represented as continuous variables together with their respective CO_2 conversion factors and are quantified inside the cube boundaries using balance equations. The material flow incorporates the immediate value stream (e.g. product, work piece, goods). It enters the cube with an assigned footprint. During the stay of the product in the cube, the cube's resource expenditures concerning this product are accumulated and assigned to an updated footprint upon exit of the product.

The ambivalence of interfaces ensures the cube's generic nature and therefore offers a lot of advantages, but it also causes one of the biggest challenges. Value streams, which are described as discrete entities, and energy flows, which are continuous by nature, must be integrated into one cube which leads to hybrid cube models. Uniting discrete and continuous modeling techniques in the cube models is one of the main challenges in implementing the methodology.

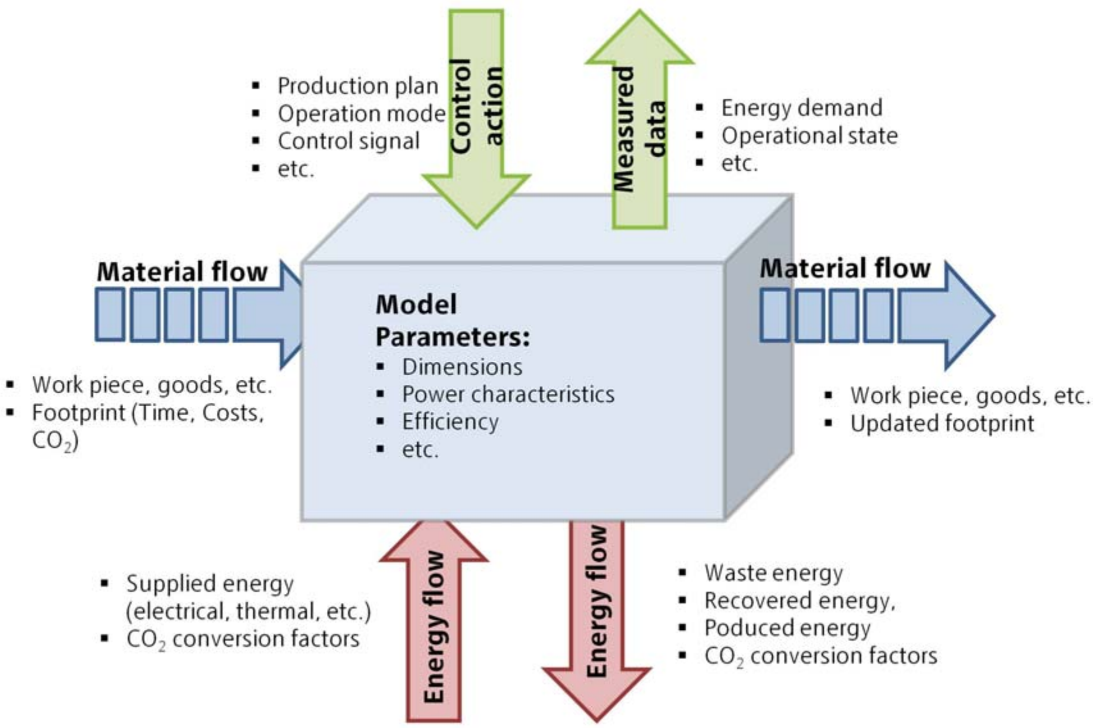

Figure 69: Overview of generic cube interfaces

In principle, every cube in a production facility (building, production plants, energy converters etc) can be represented by the generic cube model. It can however be the case, that certain interfaces can be discarded for certain types of cubes. For instance, an energy system cube (e.g. a chiller) in most cases will not be passed by a product i.e. the value stream interface is obsolete.

As mentioned above, during the stay of a product inside a cube its resource expenditures are accumulated to the product footprint. This approach to accumulate expenditures within the cubes offers the opportunity to aggregate a product footprint by applying a bottom-up approach, with the chosen cube structure defining the granularity of the result. In order to aggregate all expenditures in the plant onto the products, even if the cubes causing them are not in direct contact with the product, cubes must be able to transfer expenditure to each other. This is accomplished via the energy flows that accumulate the caused emissions, represented by a conversion factor. This requirement also implies that cubes must be of a hierarchical nature.

The congruence of system boundaries of real and virtual cubes also offers the advantage to use data from both sources to aggregate the product-footprint or other performance indicators. Given, that the monitoring system within the plant follows the cube methodology and the sensors of the measuring equipment used to capture the energy flows are placed exactly at the cube boundaries, the obtained data can be used comparatively or complementary with the simulation data. This creates the opportunity to complete the picture using different data sources, but also compare data to detect faults in either the real or virtual system.

Moreover, cubes also serve to organize the knowledge base for individual modeling tasks, by providing a concept for elementary parts of a manufacturing system that in some way contribute to the overall resource balance of the system and their possible relationships to each other. Niki Popper, partner to the research project, describes the cube approach in his dissertation as well and draws analogies to the concept of ontologies. Although, according to Popper, the cube concept does not satisfy all formal demands of an ontology, similarities in the basic concepts exist. The methodology defines objects, their properties and relationships to each other and therefore provides a knowledge base of structured domain specific information which can be put to use in multiple application cases. Furthermore, much like ontology development the cube approach is motivated by the need to understand, design and manage knowledge systems [22, Ch. 5.1]. Due to the similarity of concepts the cube approach shares many of the advantages of ontologies, as described in literature e.g. [171], [172]: Both can be an effective measure to construct knowledge bases, by organizing knowledge and providing a mechanism to understand problem statements and object statements by harmonizing specialized terminology of domain experts. Furthermore, both approaches can aid in analyzing the system description and derive models. Again they facilitate the communication between domain experts and provide a valuable support in order to determined consistency, completeness and adequacy of the model.

In order to emphasize the use of cubes as a communication tool, subcategories of cubes were introduced. Although every cube in a production facility can be represented by the generic cube model, cubes representing different parts of the system can be described with more refined properties or certain interfaces can become obsolete. Therefore, to respect these peculiarities of cube and make matters more tangible for users, a rough categorization of cube-subclasses is introduced in Figure 70. The categorization also gives a rough guideline concerning matters of granularity. As a further principle can be applied that a cube should generally possess a degree of freedom i.e. its behavior is not completely governed by the behavior of another cube.

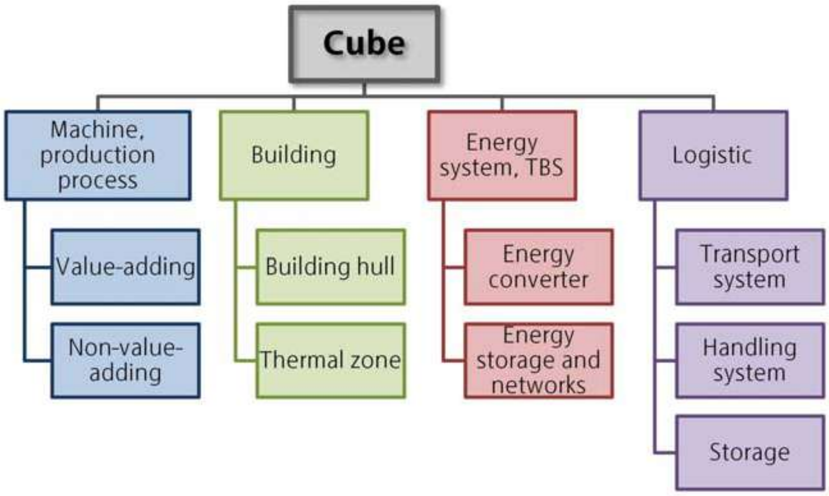

Figure 70: Categories of cubes

7.3. Preliminary Implementation Considerations

After specifying the methodology, the second main objective of Balanced Manufacturing is the development of a tool chain. Parallel with the implementation, a frame of reference management tool and a benchmark change management process based on the ISO 50001 with the objective of efficient energy management and optimization (i.e. achievement of the energy reduction targets) will be developed within the project to accompany the BaMa implementation. Some considerations concerning implementation and process have already been made and shall be briefly discussed here.

As mentioned above, one of the main challenges in implementing the cube methodology into an executable model is the hybrid nature of the cubes, i.e. the integration of discrete-event and continuous simulation models. There are few commonly known simulation environments which allow combining both modeling approaches, which showed partly very unsatisfactory test results. Furthermore, the heterogeneous domains and modeling approaches surmount the capabilities of virtually every tool. Although more flexible simulation-components or modules could be achieved by standardizing the interfaces, co-simulation is not a feasible concept for BaMa, because of restrictions concerning the implementation in the automation system. The problem was therefore approached by using the DEV&DESS (Discrete Event and Differential Equation System Specification) formalism Zeigler proposed in [173]. This formalism perfectly conforms to the nature of cubes because of its modular and hierarchical nature. More detailed elaborations concerning the application of the DEVS&DESS formalism for BaMa can be found in Niki Poppers thesis [22, p. 130].

Furthermore, first investigations and tests concerning suitable optimization algorithms for the tasks of BaMa were carried out within the project. Therefore, a test-implementation with a simple production scenario was set up and the total energy consumption was the objective function. Since the objective function is the output of the simulation, it is not possible to directly display the entire solution space through analytic functions. This fact results in the restriction, only derivative –free optimization methods can be used. Therefore, a genetic and a pattern search algorithm were selected for the test. The genetic algorithm is an evolutionary approach with inheritance of positive properties. It converges slower than the pattern search algorithm but delivers higher reliability of the results. The pattern search algorithm searches the target space according to a search pattern, which is faster but contains a higher risk to converge to local minima.

Another crucial point at reducing the modeling effort is not only to provide a high degree of reusability of the models, but also to streamline the modeling process. First experiences have been made with project partners who will implement BaMa at their production sites as proof-of-concept. One of the main challenges is the preparatory system analysis conducted in dialogue between BaMa methodology developers and domain experts on site. An approach similar to conceptual modeling frameworks, published in literature was chosen. The underlying process is oriented at the conceptual modeling framework published by Stewart Robinson in [42]. It suggests 5 basics steps to derive a conceptual model:

- Understanding of the problem situation
- Determining the modeling and general project objectives
- Identifying the model outputs
- Identifying the model inputs
- Determining the model content

Based on Robinsons general framework Tako and Kotiadis suggested a workshop structure to carry out the process of a simulation study [57]. During the initiation phase the team is assembled, basic knowledge about the system is acquired and the feasibility of the simulation undertaking is established. Afterwards the first workshop is prepared, in which the system under study is examined in detail. Problem areas and study objectives are identified and system boundaries defined. Between the first and the second workshop the outputs of the first workshop are documented and accorded between stakeholders and modeling team. In the second workshop the conceptual model is specified. Model objectives contents, scope and level of detail are agreed upon. Again, after the workshop the results are revisited and approved. Afterwards the model coding takes place. In the third workshop the domain experts are invited to critically review the results in terms of validity and performance. After an optional revision of the model in the fourth workshop the implications of the results and the implementation are discussed.

A similar process could be applied as a guideline for a Balanced Manufacturing implementation. In case of Balanced Manufacturing, where some aspects are already pre-determined by the cube structure, but many of the aspects described above, must be defined in a comparable way. As proposed by Tako and Kotiadis determining the feasibility of BaMa for the specific task at hand before launching the process seems a very obvious step. The commitment of the chosen team and the representation of domain expertise have also proven to be crucial factors for the success of the implementation.

The first workshop should be held on-sight, in order to make the production situation more tangible for the simulation team. The project has shown that it is usually almost entirely attributed to understanding of the system under study and the problem situation, mapping of the key processes of the production and the supporting infrastructure. As proposed, the next workshop concerned itself with the definition of model objectives. In case of BaMa, this translates to the questions:

- Which modules (monitoring, prediction, and optimization) are of interest concerning the use case in the company?
- Which parts of the production facility are to be integrated?

On a more specific level, it translates to:

- What are the degrees of freedom for optimization?

Based on the determined objectives, most conceptual modeling approaches suggest proceeding with the identification of inputs and outputs or system parts. Since, in case of BaMa, the in- and outputs of the system parts are mostly defined, the task at hand is to decompose the production facility into reasonable cubes (a.k.a. "cubing"). Subsequently, the phase of data collection and development of cube models can start. It also makes a lot of sense, once the model is finished, to invite the domain experts to validate the modeling results. The last workshop proposed by Tako and Kotiadis is in case of BaMa replaced by the real on sight implementation, which is a process potentially affecting and involving a large number of people. It therefore requires an accompanying change management process which will be developed in the project as well.

To conclude, it can be said that by not only providing an approach to decompose energy systems into components, but also to standardize the interfaces, the approach presented in this thesis can be modified to make simulation a feasible planning instrument in industrial software applications. One main challenge is posed by the model development, which is unique for every application. Therefore, model reusability plays a crucial role. Guru and Savory identified a combination of generic-system level conceptual model, which captures and encapsulates the component information, in combination with executable components as a promising approach to generate reusable models [51]. BaMa threads exactly this path and thereby hopes to enable manufacturing companies to balance energy efficiency and competitiveness in their continuous operation strategies.

8. Summary and Conclusion

This thesis is a summary of several years of research in the field of modeling of complex energy systems in interdisciplinary cooperation. The research question, it aims to contribute to, is how to design and operate the often rather complex on-site energy systems of consumers in the most sustainable way. A state of the art approach to answer this research question is to perform an energy system or building performance simulation, observing the energy system and the building.To draw a comprehensive picture that reflects all influences, the scope must be widened to consumers, economic aspects and the interfaces to the energy grid. In order to address these challenges this thesis develops a framework to design complex or hybrid simulations of systems focusing on energy performance related problems and an according approach for the energy system simulation itself, especially targeting interdisciplinary collaboration.

The starting point of the thesis is a comprehensive survey of the state of the art. Concepts and applications of building performance and energy system simulation are summarized and analyzed, concerning recent research trends in this field. Several of this trends, such as user representation, simulation assisted control, demand side management and lifecycle cost estimations, are potential application fields for the presented approach, as demonstrated in the application cases. Furthermore, a brief overview of co-simulation, as an important tool for simulation of complex systems is given. A special focus was also put on the theory of modeling and simulation processes and conceptual modeling. Surprisingly little literature exists concerning approaches to conceptual modeling despite its fundamental impact on the success of a M&S task and none of the proposed approaches seemed to match the particular needs of energy system modeling.

In order to fill this gap a reference model for energy system modeling is proposed based on methods developed by the previous research analyzed in the state of the review. The reference model includes a description of the process, leading from a research question or problem field to an executable model. It furthermore suggests a conceptual model representation specifically targeted at energy system models. The reference model was designed aiming at modeling processes in interdisciplinary collaborations, in which the reuse of existing domain specific modeling, simulation and tool knowledge as well as executable models is of interest. This reuse interest is in most cases motivated by considerations of modeling effort vs. model and simulation life span. Therefore, the proposed approach does not only rely on the top-down approach of model decomposition, as suggested in most publications concerning conceptual modeling, but also takes the needs of domain experts concerning reuse of models and tools as well as knowledge representation into account.

After the reference model, the energy system model itself is regarded in more detail. The specific challenges concerning the energy system model rising from the embedment in a complex simulation environment are discussed. Based upon these considerations a model structure for the overall energy system model to match the reference model is suggested. It fuses deductive modeling approaches at system level with inductive approaches at component level. This approach reflects that components, although of varying characteristic according to type and manufacturer, are representations of the same basic concept, which can be implemented through inductive models, because they can depict an infinite number of variations by altering the parameterization. On the other hand the system configuration usually is a unique solution and therefore, the deductive approach fits well. Furthermore, validation and verification techniques matching the chosen modeling approaches are suggested and a library in accordance with the findings is introduced.

In order to illustrate the proposed approach and proof its feasibility, two application examples, developed in two interdisciplinary research projects with a different scope are presented. One example deals with the development of a software planning tool for optimization of the energy performance of manufacturing companies. This application case features a classic M&S application (analysis) but a rather challenging modeling task, due to the requirement of universal applicability to all kinds of manufacturing companies. The other project aims at the implementation of a model predictive controller in an office building in order to minimize the heating and cooling energy demand. In this case the modeling task is fairly well defined but the implementation is challenging, because it has to integrate hardware and simulation, and meet the requirement of real-time application. Both projects could be concluded successfully with the help of the presented approach, which was also developed in the course of the projects.

Finally, the thesis presents another project that deals with energy efficient production, but in this project the goal is to develop a simulation based software tool chain for predicting and optimizing the energy efficiency of production plants. Therefore, the simulation implemented in the tool chain has a considerably longer life span and needs to be very modular, in order to be able to assemble new instances with limited effort, because every software implementation calls for a new model. In this case the reusability of existing models is less of an interest than the internal reusability. Therefore, for this project an alternate approach, with very rigid decomposition into formalized modules is chosen. This eliminates the possibility for model or tool reuse almost entirely and even calls for programming a tailored simulation environment. This effort only pays off because of the long life span and the gained internal reusability.

So, ultimately there is always a tradeoff between reusability of existing elements and internal reusability, which must be reflected in the chosen modeling approach. The stricter the top-down decomposition is applied, the more internal reuse can be gained but also the more effort is caused by the modeling process and implementation. On the other hand the more bottom-up aspects are integrated into the modeling, the more reusability of existing models is gained and effort avoided.

By proposing a framework to generate models to design complex or hybrid simulations of systems focusing on energy performance related problems this thesis tries to minimize the effort for modeling and therefore, reduce the barrier to applying modeling and simulation technologies for solving holistic energy efficiency optimization problems. Lowering this barrier will hopefully contribute to the knowledge on how to design and operate complex on-site energy systems of consumers in the most sustainable way. For future research and development the ultimate goal would be to further minimize the modeling effort through automated model generation. This would hopefully lead us closer to solving society's energy and emission problem by exploiting energy efficiency as our biggest energy resource.

> *The Stone Age came to an end, not because we had a lack of stones, and the oil age will come to an end not because we have a lack of oil.* [174]
>
> -Sheik Zaki Yamani, Saudi Arabian oil minister 1962 – 86

Appendix

Nomenclature

Abbreviations

Abbreviation	Text
BaMa	Balanced Manufacturing (research project)
BCVTB	Building Controls Virtual Test Bed (software)
BIM	Building information modeling
BPS	Building performance simulation
CFP	Carbon footprint of products
CHP	Combined heat and power
CM	Conceptual model
COI	Community of interest
COP	Coefficient of Performance
CoOpt	Koordinierte Optimierung von erneuerbarer Energie in Netz und Gebäude bei Planung und Betrieb (research project)
DESS	Differential Equation System Specification
DEVS	Discrete Event System Specification
DSM	Demand side management
ERP	Enterprise resource planning
HIL	Harware-in-the-Loop
HTF	Heat transfer fluid
HVAC	Heating, ventilation and air conditioning
IC	Information component
ICT	Information and communication technologies
INFO	Interdisziplinäre Forschung zur Energieoptimierung in Fertigungsbetrieben (research project)
LCBA	Life Cycle Cost and Benefit Analysis
KPI	Key performance indicator
MES	Manufacturing execution system
MPC	Model predictive control/controller
M&S	Modeling and simulation
PC	Physical component
PCM	Phase change material
PV	Photovoltaic
ROI	Return on Investment
SME	Subject matter expert
SoS	Systems of systems
TBS	Thermal building system
UML	Unified modeling language
V&V	Validation and verification

Mathematical Symbols - Latin

Symbol	Unit	Definition
A	m^2	Area
a_i, b_i, c_i	–	Coefficients
CCF	--	Cooling capacity factor
COP	--	Coefficient of Performance
C_p	J/K	Heat storage capacity
c_p	J/(kg K)	Specific heat storage capacity
$C_{p_{bat}}$	Ah	Peukert Capacity
c_T	1/K	Temperature factor
$CVPF$	--	Cooling volumetric performance factor
E	kg/s	Fuel consumption
f	--	Volumetric fraction
g	--	Transmittance
H	h	Nominal charging time
h	J/kg	Specific enthalpy
h_{g0}	J/kg	Specific enthalpy of saturated steam at water 0°C
h_{gw}	J/kg	Specific enthalpy of saturated steam at water inlet temperature
HIF	--	Heat input factor
$HMFC$	--	Heat medium flow correction
$HVPF$	--	Heating volumetric performance factor
HWE	--	Hot water efficiency
h_{sw}	J/kg	Specific enthalpy of saturated humid air at water temperature
I	A	Electric current
I	W/m^2	Solar irradiation
i	Varying	Input variable
k	$W/(m^2 K)$	Heat transfer coefficient
k	--	Peukert exponent
k_0	--	Cooling tower constant
$K_1(50°)$	--	Angle factor for 50° incidence angle
k_D	--	Pollution factor
k_T	--	Temperature factor
k_Θ	--	Angular factor
Le	--	Lewis number (dimensionless number)
LF	--	Load factor
$\dot{m}$	kg/s	Mass flow
n	1/h	Air exchange rate
o	Varying	Output variable
P	W	Power
$\dot{Q}$	W	Heat flow
T	K	Temperature
t	s or h	Time
U	V	Voltage
U	W/K	Heat transfer coefficient of total surface
u	m/s	Fluid velocity

v	$\mathrm{m/s}$	Velocity
X	$\mathrm{kg/kg}$	Water load
x	Varying	State variable

Mathematical Symbols – Greek

Symbol	Unit	Definition
α	W	Heat transfer coefficient
η	–	Efficiency
θ	°	Solar incidence angle
λ	–	Air ratio
ρ	$\mathrm{kg/m^3}$	Density
τ	s	Time constant for mixing
ϑ	°C	Temperature

Mathematical Symbols – Subscripts

Symbol	Unit	Definition
a		Algebraic
abs		Absorber
ae		Algebraic equation
air		Air
amb		Ambient
$cold$		Referring to flows for refrigerating purposes
$coll$		Collector
$cond$		Condenser
$condu$		Conductive
$conv$		Convective
$cool$		Referring to flows for cooling purposes
d		differential
dae		Differential algebraic equation
el		Electric
$evap$		Evaporator
f		Fluid
$gain$		Gains
gen		Generator
$heat$		Referring to flows for heating purposes
HTF		Heat transfer fluid
in		Incoming/inlet
inf		Infiltration
int		Internal
$loss$		Losses
mix		Mixing
nom		Nominal

out	Outgoing/outlet
PCM	Phase change material
PV	Photovoltaic
$room$	Room
RL	Return line
seg	Segment
SL	Supply line
$storage$	Storage
$TABS$	Thermally activated building system
tot	Total
w	Water
wh	Waste heat
$wall$	Wall
$window$	Window
$zone$	Thermal Zone

List of Figures

List of Tables

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Ines Leobner

ines.leobner@tuwien.ac.at, +43 650 2350050

Personal Data

Date/Place of Birth: 13 April 1983, Linz, Austria
Residence: Schleifmühlgasse 15/5, 1040 Wien
Citizenship: Austria

Professional Experience

Research Assistant, Institute for Energy Systems and Thermodynamics, Vienna University of Technology, Vienna, Austria (4.2010 to present), Institute for Production Engineering and Laser Technology (1.2014 to present)

- Fields of research: Energy efficiency in manufacturing industry, building energy systems
- Teaching: Fundamentals of thermodynamics, building energy systems, supervision of theses

Assistant of Vice-Chancellor for Infrastructure Management and Development, Vienna University of Technology, Vienna, Austria (5.2008-3.2010)

Technician for measurement engineering and process control, Ing. Erwin Mühlegger GmbH, Traunkirchen, Austria (Location of Work: Germany) (2004-2007 temporary)

Internship, Jenbacher Energiesysteme AG (now: GE Jenbacher GmbH & Co OHG), San Sebastian de los Reyes, Madrid, Spain (7.2003)

Education

PhD Studies in Mechanical Engineering, Vienna University of Technology, doctoral college Energy Systems 2030 (5. 2010 - 12. 2015)

Diploma Studies in Mechanical Engineering, Vienna University of Technology, special field: Energy Systems (10. 2001 – 4. 2010)

- Diplom-Ingenieurin für Maschinenbau (Master of Science in Mechanical Engineering) (4. 2010)

General qualification for university entrance, Bundesrealgymnasium Kirchdorf an der Krems, Austria (6. 2001)

Research Projects:

Balanced Manufacturing (BaMa), funded by Austrian Research Promotion Agency within the Program e!Missi0n+.at, 2014 – 2017

Coordinated Optimization of Renewable Energy in Grids and Buildings for Planning and Operation – SmartCityGrid:CoOpt (Koordinierte Optimierung von erneuerbarer Energie in Netz und Gebäude bei Planung und Betrieb), Funded by Austrian Research Promotion Agency within the Program New Energies 2020, 2012 – 2014

Energy Systems 2030 - ENSYS 2030, Doctoral college funded by Vienna University of Technology, 2010 – 2013

Interdisciplinary Research on energy efficiency in manufacturing enterprises - INFO (Interdisziplinäre Forschung zur Energieoptimierung in Fertigungsbetrieben), Funded by Austrian Research Promotion Agency within the Program New Energies 2020, 2010 - 2013