



Article

Holistic Simulation Approach for Optimal Operation of Smart Integrated Energy Systems under Consideration of Resilience, Economics and Sustainability

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Abstract: The intermittent energy supply from distributed resources and the coupling of different energy and application sectors play an important role for future energy systems. Novel operational concepts require the use of widespread and reliable Information and Communication Technology (ICT). This paper presents the approach of a research project that focuses on the development of an innovative operational concept for a Smart Integrated Energy System (SIES), which consists of a physical architecture, ICT and energy management strategies. The cellular approach provides the architecture of the physical system in combination with Transactive Control (TC) as the system's energy management framework. Independent dynamic models for each component, the physical and digital system, operational management and market are suggested and combined in a newly introduced co-simulation platform to create a holistic model of the integrated energy system. To verify the effectiveness of the operational concept, energy system scenarios are derived and evaluation criteria are suggested which can be employed to evaluate the future system operations.

Keywords: cyber physical energy system; cellular approach; transactive control; smart integrated operation; dynamic modeling; co-simulation



Citation: Hoth, K.; Steffen, T.; Wiegel, B.; Youssfi, A.; Babazadeh, D.; Venzke, M.; Becker, C.; Fischer, K.; Turau, V. Holistic Simulation Approach for Optimal Operation of Smart Integrated Energy Systems under Consideration of Resilience, Economics and Sustainability. *Infrastructures* **2021**, *6*, 150. <https://doi.org/10.3390/infrastructures6110150>

Academic Editor: Isam Shahrour

Received: 30 September 2021

Accepted: 18 October 2021

Published: 23 October 2021

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1. Introduction

In order to reach the climate goals of the Paris Agreement, to which a large part of the world's community are committed, it is necessary to achieve a high degree of decarbonization across the energy sectors [1]. In Germany, the changes to the Federal Climate Protection Act in August 2021 reaffirmed these efforts, made them more concrete, and set higher goals [2]. The strategy for achieving these goals is the installation of renewable energy sources, consisting mainly of wind turbines and solar power plants [1] in the electrical energy system. Such intermittent renewable sources are highly dependent on the weather conditions, mainly solar radiation and wind speed. Therefore, they cannot be operated like conventional fossil power plants, but require high degrees of flexibility while balancing generation and consumption within the energy system [3]. Furthermore, these flexibilities depend upon the new operational strategies, digitization and cooperation of the sector coupled energy system, e.g., making full use of the flexibility within production and consumption, named "prosumption", in the coupled heat, gas and electric grids. In other words, a cyber physical system for the sector coupled energy system or, as it is referred to in this paper, an Smart Integrated Energy System (SIES), is required to generate and make use of these flexibilities. Figure 1 illustrates the basic connection of the three energy sectors.

Information and Communication Technology (ICT) connects the physical technologies to the control, which represents the management strategies in future SIES.

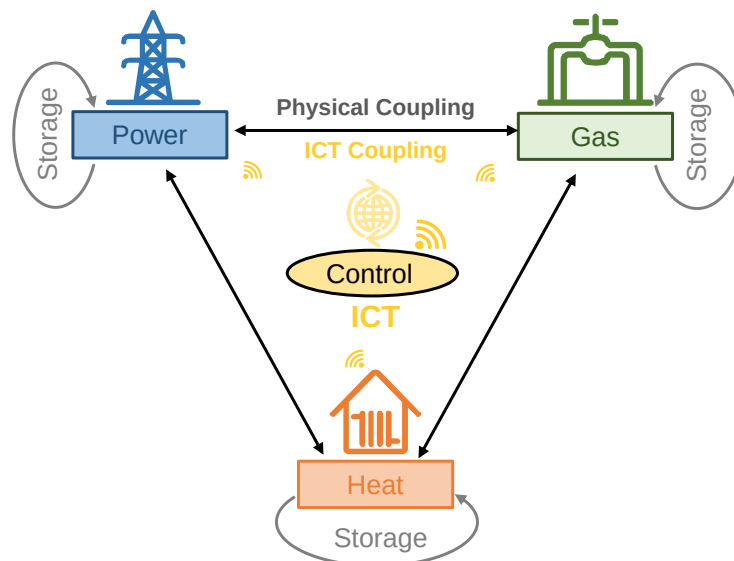


Figure 1. Physical and ICT coupling of energy sectors.

In current research, there are a lot of different approaches trying to define such an SIES architecture. One promising approach for the architecture of SIES is the Cellular Approach (CA) conducted by the German VDE [4]. In the CA, the conventional energy system is split into cells of different levels. Every cell in the CA has its own form of cell management in the form of a cell manager that monitors and orchestrates the local generation and consumption. This decentral and hierarchical operation allows for the acquisition of the required flexibility to locally maintain the balance of load and operate resilience strategies in the case of failures. Since flexibility is mainly a product of the end-user, e.g., companies or households, which are flexible in the use of their appliances, a smart market system is needed to collaborate with the SIES. One of the commonly discussed methods for this purpose is the use of smart local markets on the basis of Transactive Control (TC) [5,6].

These architectural specifications are intensely discussed in the literature. Relevant projects in this research field are, for example, the SINTEG project C/SELLS [7], the research project ZellNetz2050 [8] from the university of Wuppertal, which is a holistic approach for designing, modeling and evaluating these future SIES, and a concept for holistically evaluating an SIES in terms of sustainability, resilience and economic efficiency, which represent gaps in research. Therefore, the goal of this work is to contribute with:

- An innovative operational concept for SIES;
- A framework for the holistic simulation of SIES;
- Scenarios and evaluation criteria for the optimization of the operation of an SIES.

2. State of the Art

Future energy systems will be more strongly interconnected in different domains. Sector coupling connects different energy sectors to make use of spatio-temporal distributed energy resources and to combine the intermittent energy supply with controllable loads and storages, referred to as flexibility (Section 2.1). In the context of operational management, the energy system is monitored on the one hand, and setpoints for active elements, e.g., storages, electric vehicles or heat pumps, are calculated for the optimal exploitation of flexibilities on the other hand (Section 2.2). This requires detailed dynamic models and a wide availability of data (Section 2.3). While physical coupling can lead to an enhanced system stability, digital interconnection with the usage of information and communication

technology (Section 2.4) as a prerequisite for innovative operational concepts can endanger the stability due to vulnerability to cyber attacks, dependency on stable energy supply for digital infrastructure and a higher risk of failure. Therefore, a detailed modeling is necessary to investigate advantages and restrictions through the utilization of ICT coupling technologies. This transformation and innovation also takes place in the design of new integrated market mechanisms (Section 2.5) and physical topologies in the energy system (Section 2.6). Regional and supra-regional marketplaces can also be used for the procurement of ancillary services and thus be linked to the physical structure (Section 2.7).

2.1. Sector Coupled Energy Systems

Decarbonization is one of the main targets of the energy economy in order to reach global climate targets. In this regard, fossil energy carriers are to be substituted increasingly by distributed energy resources (DERs), which mainly provide energy in the form of electricity, e.g., by photovoltaics (PVs), wind energy, and hydro power. There are inherent economic reasons for a constantly rising share of electricity to about 65% in 2050, mainly versatility and energy efficiency compared to fossil fuels [9]. Nevertheless, energy carriers will still be important in mostly all energy sectors. These include, for example, hydrogen and methane as energy storage, fuel for transportation and other energy carriers for the industry.

As conventional power plants are placed in areas with high electricity demand, DERs will emerge in areas with high solar irradiation and much wind, which will be mostly at other locations due to economic reasons. Moreover, DERs rely on intermittent primary energy. Consequently, there is a greater need for flexibility on the consumption side. These two aspects together with a still diverse energy demand lead to spatial and temporal challenges in energy provision, where sector coupling (SC) will play a promising role in the future [10]. In this context, in SC, one can distinguish between the main three energy sectors electricity, heat and gas on the one hand and between the application and demand of transportation, households, services and industry on the other hand. The major reason for SC is the reduction in greenhouse gas emissions [11]. Moreover, the strong interconnection of formerly individual sectors creates a wide range of possibilities for the application of complex energy conversion chains in order to optimize the operation of such energy systems.

2.2. Operational Optimization of Sector Coupled Energy Systems

The operation of sector coupled energy systems allows to make use of a variety of possible energy conversion chains in order to reach formerly defined setpoints of energy-producing units while optimizing criteria based on energy-political targets, namely sustainability, supply safety and economic efficiency.

Many operational optimization approaches mainly consider operational costs. In research, a vast amount of different models and optimization tools exist with different tasks and spatio-temporal resolutions in focus [12]. In electrical power systems, Optimal Power Flow (OPF) is one established procedure to define optimal setpoints of power plants to fulfill a defined energy demand [13]. This procedure is also known for gas and heating networks with the goal of minimizing energy costs, since the mathematical formulation of the underlying load flow calculation is similar [14]. Ref. [15] suggests a method for the optimal operation of intersectoral loads and electrical energy storages in an energy hub system considering stochastic uncertainties in the DER feed-in. Energy hubs as an interface between the producer and consumer and a multi-vector system [15], in which energy flows between different entities such as from power to gas and storages are not predefined, are optimized regarding their structural compositions in a similar way in [16]. Multi-carrier microgrids, compared to traditional microgrids extended by conversion facilities, are optimized in [17] regarding operating costs using transactive energy mechanisms. Even if the goal of cost reduction inherently takes the goal of sustainability into account, a stronger focus must be specifically placed on aspects of sustainability and resilience.

Security constrained economic dispatch is one established procedure, which considers line loads during OPF [18]. Additionally, OPF can be extended by aspects of sustainability using a multi-objective optimal power flow [19].

2.3. Dynamic Modeling of Physical Energy Systems

For the purpose of operational optimization, suitable models are required. In the modeling of power systems, steady-state and dynamic modeling is widely established. Steady-state models are well-suited for system analyses for a long time span, e.g., for one year. It is assumed that processes in every simulated time step are in a state of equilibrium, which reduces the computational effort significantly. The use cases are, for example, the long-term optimization of the composition of energy-producing units with constraints defined by sustainability and the subsequent solving of unit commitment and economic dispatch problems, as it is achieved in the project REMod-D [20]. Typical time slice lengths for the temporal data input range from years to weeks dependent on the time scope. The finer the temporal resolution, the higher the modeling accuracy, especially for systems with high shares of renewable energies [21]. Ref. [12] gives a broad review of current energy system modeling tools.

When it comes to short-term operational energy planning, the occurring error by modeling physical processes in the quasi-stationary state is high. Influences from systems which are not balanced cannot be tackled in this way, resulting in an overestimation of the baseload and an underestimation of needs for flexibility [21]. Taking into account the dynamic process requires mathematical modeling using differential algebraic systems (DAEs) for physical processes and proceeds over a much shorter time scale, below one hour [22]. In order to design operational management functions with respect to the system's resilience and analysis of interactions, the dynamic modeling of the physical components becomes inevitable [23,24]. Moreover, dynamic modeling is required in order to design coordinated control strategies and analyze the system stability with effects acting in the same time scope across all relevant sectors. At TUHH, the TransiEnt-Library [25] was developed, which is still under active development. The library comprises a wide field of physical models for the energy system, mainly in the three energy sectors, power, heat and gas, and is written in the open object-oriented acausal modeling language Modelica [26]. Another tool for modeling and optimizing energy systems dynamically is PyPSA, developed in Python at the Karlsruhe Institute of Technology [27].

2.4. Modeling of ICT

The simulation of the ICT addresses the new challenges in future energy systems. These range from the increasing the load on the power grids to the diversity and intermittency of the production structure [28]. Through methods such as the management and analysis of power grids, the simulation of ICT aims to contribute to resilience and digitization in order to meet the expectations of new energy systems and to ensure their protection against external and internal threats to cyber security [29]. Ref. [30] shows how ICT-relevant data affect the operational management, e.g., state estimation, in SCADA applications. For the aspect of resilience, ref. [31] presents a list of fields of action in regard to the identified security problems and elaborates on corresponding measures. A similar approach has been conducted by Appelrath et al. in order to identify the action points needed en route to the aspired digitization of ICT systems [28].

In the decoupling of hardware and software in digital systems in the subject of variability regarding the development of new functionality, possibility to react to cyber attacks and adaption to new environments, virtualization presents an important opportunity. Ref. [32] emphasizes Grid Function Virtualization (GFV) as one possibility to make use of virtualization technology in the power system. Ref. [33] specifically investigates the contribution of virtualization to adapt grid services during disruptive events to enhance reliability and resilience.

The simulation of these aspects requires the integration of the ICT layer in the modeling of future energy systems. Ref. [34] identifies six possibilities for the simulation of communication within energy systems. Determining the performance of the communication structure directly using individual network simulators is the simplest method to achieve this [34]. However, this method cannot fully mirror the impact of coupled communication on the the energy system dynamics [35,36]. Another option is to develop a new simulator that combines physical dynamics and communication networks [34]. This approach is expensive and time-consuming [34]. Another fundamental approach is co-simulation, as it integrates the perspectives of the physical system and communication in a cross-disciplinary way with less time and cost. To co-simulate both the physical system and the communication networks, ref. [34] presents two main methods, the extension of a particular simulator and the co-simulation of individual simulators.

The first method of co-simulation considers the extension of a simulator in order to integrate the dynamic characteristics of the physical system and the communication networks. This method is divided into two categories: approaches for extending communication network simulators and approaches for extending energy system simulators. The extension of OPNET by Tong et al. is an example of the extension of communication network simulators, where the dynamic simulation of the physical system is an individual module within OPNET that is called whenever a calculation of the dynamics of the physical system is required [37]. Other communication simulators allowing the emulation principle such as OMNeT++ can also be used to realize this co-simulation approach. This method is only used for the simulation of short and simple scenarios because it cannot effectively cope with high levels of complexity in the physical system or the communication networks [38].

The second method co-simulation introduced in [34] consists in the integration of existing simulators for a specific domain through one tool. This allows one to use the advantages of the different simulators. However, time-based physical system simulators and event-based communication network simulators require the development of synchronization and data exchange modules within the co-simulation tool in order to guarantee communication between simulators. Several co-simulation platforms are listed and compared in [34]. In [39], two different co-simulation methods, namely Mosaik and High-Level Architecture (HLA), are compared. Co-simulation enables the integration of further simulators such as a market simulation.

2.5. Market Mechanisms

The integration of market models within energy system simulations allows a more realistic and sophisticated modeling of the involved actors' behaviors [40]. Especially in future energy systems, within the increasing importance of DERs and thus a shift from mostly passive consumers to a large number of active market participants, the design of adequate market mechanisms plays a crucial role in realizing the potential of such complex systems [41]. The challenge of employing flexibility in generation, consumption and storage depends on the widespread acceptance of market structures that create incentives to participate in and contribute to the system [42]. In view of the conflicting overall objectives of sustainability, resilience and economic efficiency, a holistic energy system simulation including a market model enables sophisticated solutions to be found with consideration of these interdependencies. However, adequate market mechanisms do not only pertain to economic factors. Other factors and objectives of related parties are reflected in the market behavior and can be further facilitated through monetization [43], as was carried out, for example, with the trading of CO₂ certificates. An important notion regarding future energy markets is the transition from energy suppliers to aggregators with a higher flexibility potential [44]. The existing literature presents different approaches for modeling energy markets. These include optimization models from a central planner's perspective, agent-based simulation models and game theoretic models, each with different implications for the model's scope and purpose [45,46].

2.6. The Cellular Approach

The CA is a novel concept for the hierarchical structuring of SIES in a Cellular Energy System (CES) consisting of Energy Cells (ECs). Research related to the CA has been conducted for over a decade. The first major milestone in the history of the CA was reached by the German VDE in 2015 [47] with the goal to investigate and provide a concept for sustainable energy supply systems in a long-term perspective with high-density renewable energies. The CA is still under investigation and research in this area is still under way.

The structural concept referred to in this publication is mainly based on the newest research contributed by the German VDE [4]. As mentioned before, the CES is built as a mesh of EC. “Energy Cells consist of the infrastructure for different forms of energy in which, through management of the energy cell in possible coordination with neighboring cells, generation and consumption across all available forms of energy is organized” [4]. These EC are non-equally distributed over the whole SIES landscape.

In the German VDE approach, there are five different levels of EC, which in the following will be referred to as EC level 1 to EC level 5. EC levels 1 and 2 consist of high-voltage and high-pressure transmission grids and contributing appliances. EC levels 4 and 5 contain low-voltage and high-pressure grids as well as single households or small companies. Each EC of level N consists of multiple EC of level $N + 1$. Other definitions by Flatter et al. divide the cells into the levels A to C by merging cell levels 1 and 2 as well as 4 and 5 together [8].

In this regard, Figure 2 shows two levels of the CES. The wider EC is a level 3 EC and consists of six ECs of level 4. The physical coupling technologies, including the electric, gas and heat grids, are indicated by the background color of the cells and are not shown in more detail in the figure for reasons of clarity. It can be seen too that the digitization in this architectural concept is assumed to be fully completed in the low voltage grid and each asset has the possibility to communicate with their local cell manager. The cell managers can communicate with the cell managers of their respective upper and lower EC levels.

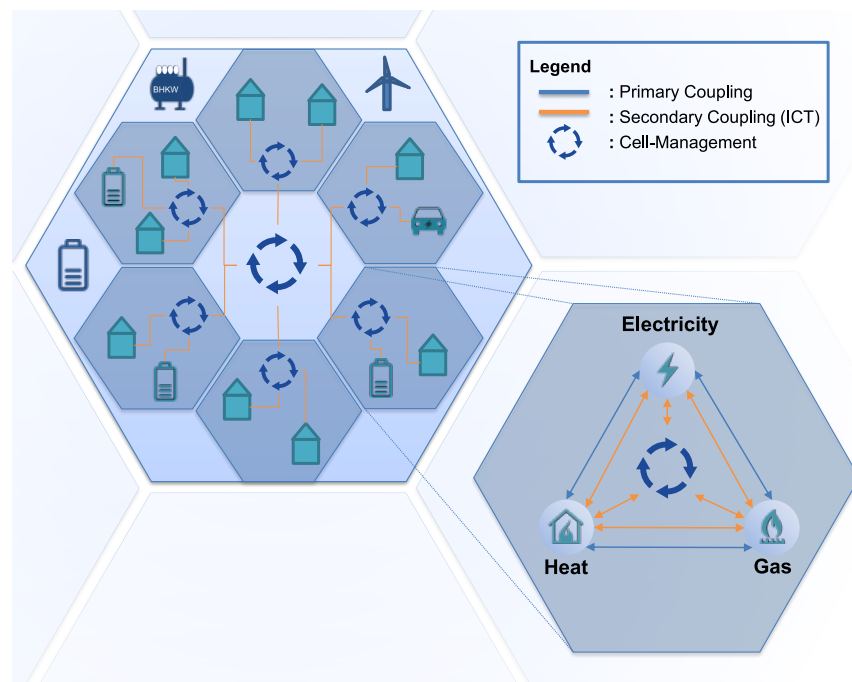


Figure 2. Cellular energy system.

One important aspect which has to be named alongside the CA is the subsidiarity principle. This principle is one of the key aspects of the CA and means that every cell management strategy in general has to balance the mismatch of production and consumption inside their own EC as a priority. Therefore, cell management needs to have access to flexibilities in order to achieve this requirement.

2.7. Transactive Control

In addition to a concept for the architectural design of energy systems, a concept regarding the system's energy management is required. In the context of digitized smart grids with a high number of DERs, TC is a concept that provides the means for employing decentralized flexibility with the aim of improving the system's efficiency and reliability [5,6]. In accordance with the widely adopted definition by the GridWise Architecture Council of Transactive Energy, "a system of economic and control mechanisms that allows the dynamic balance of supply and demand across the entire electrical infrastructure using value as a key operational parameter" [48], this is achieved by implementing control mechanisms that operate on the basis of markets. Transactions between large numbers of decentralized actors are coordinated through frequent exchanges of information and thereby finding equilibriums [49]. By defining the boundaries, rules and pricing schemes in which the market participants' negotiations are set, the market or grid operator influences the individual objectives in favor of system objectives [5]. Accordingly, the application of transactive energy systems can achieve objectives such as frequency regulation and control, congestion and voltage management or grid balancing without exerting any centralized control actions [49]. An important method in this regard is the distribution locational marginal pricing scheme, which means that energy prices are dependent on local resilience and reliability issues [50].

In line with the subsidiarity principle, such TC markets are suitable in the form of local energy markets in addition to larger wholesale markets in order to manage and control the grid using local flexibility offers [44,51]. There are two basic implementing methods in regard to the information exchange process for finding equilibriums. The iterative information exchange-based method comprises a number of iterations of market bids and responsive price signals and is thus used in the day-ahead scheduling phase. In the intraday or real-time control phase, the one-time information exchange-based method is more suitable, given the short-term nature and the lower number of bidding options [49].

3. Concept for Optimal Operation by Holistic Modeling of Smart Integrated Energy Systems

In this section, the concept for the optimization of the operation shall be introduced. The following approach is based on holistic modeling, meaning that physical and ICT coupling technologies are modeled for investigation and the optimization of the operation, as well as market mechanisms and their effects. In order to optimize the system's operations, a methodological process is given in Section 3.1. Section 3.2 presents the basic operational concept. Section 3.3 concludes this chapter by going into detail with respect to the simulation concept, which is a central part of the process.

3.1. Methodology

This paper's approach for optimizing the operation of SIES is based on four key components, which are scenarios, simulation models, evaluation and optimization steps.

In order to model future SIES, one needs to define the technical, political and structural conditions. Therefore, the development of corresponding scenarios is a requirement in order to build realistic models. In this work, the scenarios are conducted for the reference year 2050. In accordance with Figure 3, the scenarios are the basis for the modeling process and define a framework for the subsequent simulation. In order to define and distinguish scenarios, a set of key aspects, referred to as features of the SIES, is needed. These features represent the technical, economical and political situations.

For each scenario, the simulation is designed under the consideration of an adequate set of operational concepts for the grid architecture, respectively. Since holistic modeling is the goal of this work, the co-simulation of the physical system, ICT and market models is required. A more detailed insight into the simulation structure is presented in Section 3.3.

The next step is the application of evaluation criteria from the perspective of resilience, economic efficiency and sustainability. These criteria are needed to analyze the simulation outputs for a representative simulation period of four weeks and thus provide a guide for optimizing the operational concept with respect to current political objectives. In order to employ the evaluation in an objective and structured way, a systematic approach for merging a variety of different indicators into an overall system evaluation is implemented.

The final component is the identification and implementation of adequate optimization measures on the basis of the system evaluation. The possible subjects of optimization are predefined system parameters and processes, such as, for example, state estimation algorithms. Such adaptations only take place within the operational concept or the ICT structure, since topology alterations in regard to the physical coupling model are not in the scope of this work. After the implementation, another iteration of the process follows with the aim of assessing the effectiveness of the applied measure and possibly identifying further optimization steps.

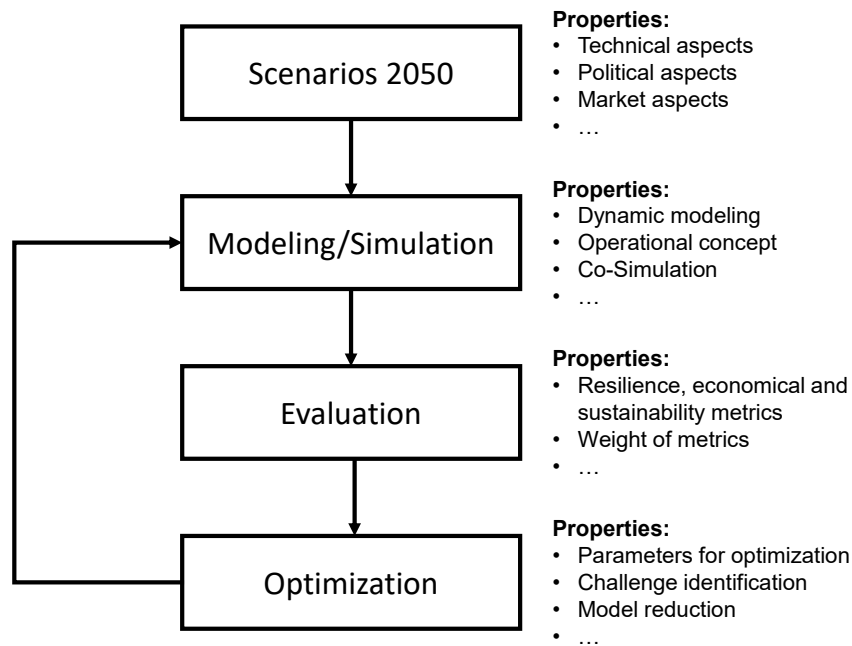


Figure 3. Cyclic method for scenario-based holistic modeling and the evaluation-based optimization of operational concepts.

3.2. Operational Concept

The methodological process described in the previous section revolves around the operation of an SIES. In order to simulate and further optimize the operation, a basic operational concept is required. This concept specifies the system processes and the roles of the involved actors. Two different stages of operation are distinguishable with respect to the underlying processes. The day-ahead operation regulates the planning process at a fixed point in time each day for the upcoming day from 00:00 to 24:00. The intraday operation consists of continuous processes to consider real-time and short-term developments and to efficiently manage the forecast deviations of the day-ahead planning. The operational concepts are presented in Figures 4 and 5, respectively.

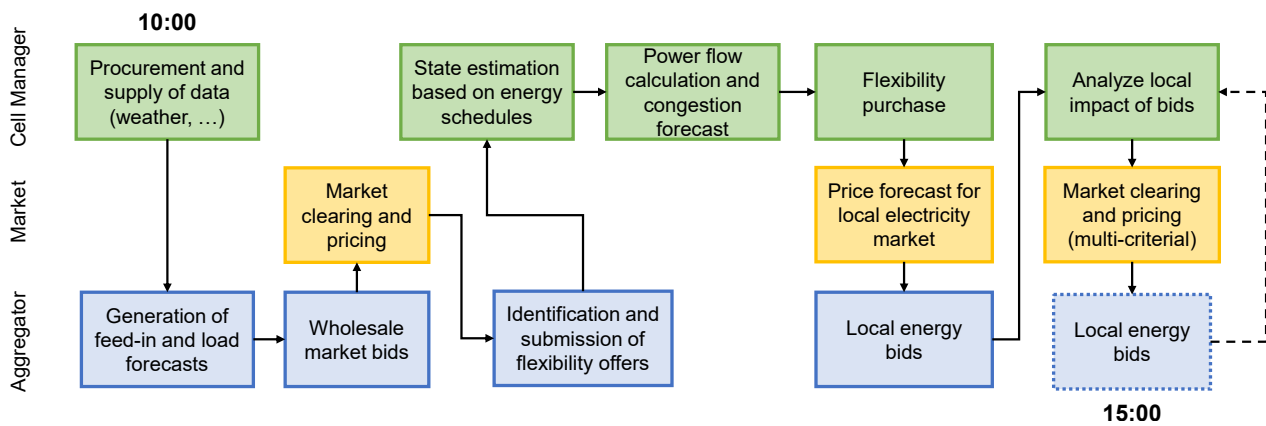


Figure 4. Operational concept for the day-ahead process.

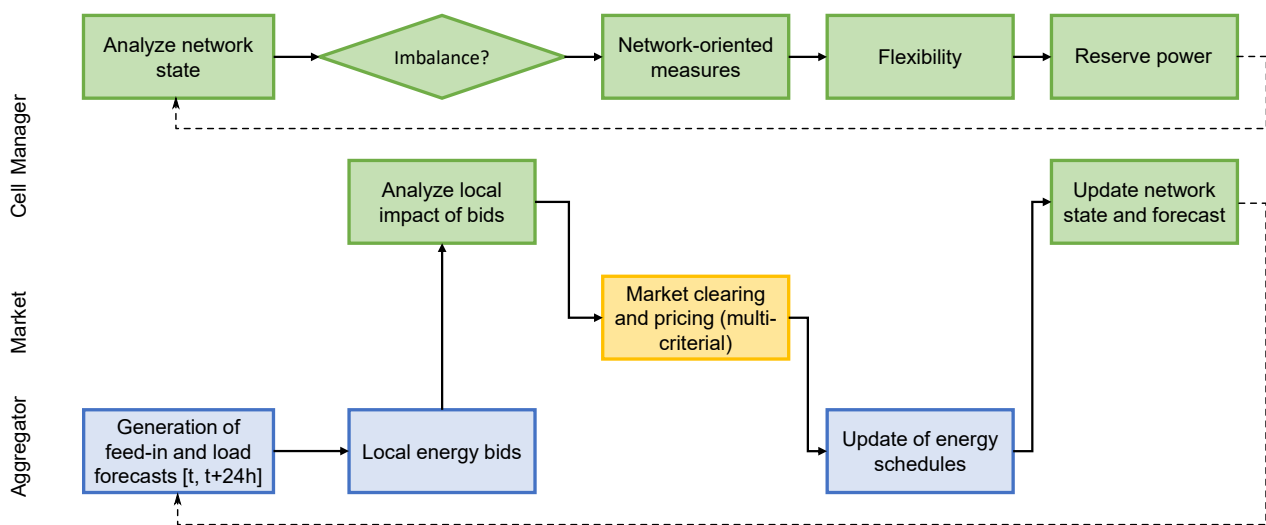


Figure 5. Operational concept for the intraday processes.

These concepts assign roles and functions to three major types of actors in EC levels 3 and 4: cell managers, market operators and aggregators. Aggregators act as free agents of minor actors in EC level 4 in order to perform the complex task of efficient and effective energy management for a multitude of households. This includes energy market participation on behalf of their clients. In addition to the wholesale day-ahead market, local energy markets are implemented in accordance with TC. These local markets are linked to the cell control in the sense that the market mechanisms and the inherent pricing schemes take input resulting from the respective cell managers’ network analyses into account. Consequently, under consideration of the current technical circumstances, the cell managers create incentives to employ the flexibility of DERs in line with local system objectives.

The day-ahead concept consists of three different phases. In the first phase, a wholesale energy trade is conducted in which the aggregators from all ECs of level 4 take part. After the wholesale market clearing, cell managers from EC level 3 have the opportunity to purchase flexibility from local aggregators. An iterative energy market in EC level 3 constitutes the third phase in which the market clearing mechanisms consider multi-criteria inputs from the respective cell managers and thus reward bids that support the resilience of the local grid or contribute to sustainability. The intraday operational concept consists of a similar local energy market. However, only one iteration of the bidding and market clearing process is used for the respective trading intervals.

3.3. Simulation

In order to create a simulation setup, the architecture of the SIES needs to be defined initially. The concept of CES is determined to be appropriate for this work’s purpose. Therefore, the topology in the dynamic physical energy system model shall be modeled in four different levels of cells (ECL 1–ECL 4). Additionally, the relevant ICT infrastructure is to be modeled in order to enable the operation of the cellular energy system in terms of cell management and market coordination. To achieve this and to make full use of the advantages of dynamic simulations, a co-simulation between the dynamic physical and ICT model with a high temporal resolution is to be designed. The holistic simulation also integrates the cell management model as well as the market model. However, the temporal resolution prerequisites differ within the different subsystems, since market operations in the scope of this work do not occur in the range of seconds or microseconds.

In Figure 6, the relation between the different models is given in relation to the co-simulation platform. A general distinction can be made between dynamic models on the left side and the operational processes and their respective models on the right side. The dynamic models are mainly characterized by the architecture and the input given by scenarios. The operational models contain complex algorithms and consider possible structural designs for markets and regulations. Thus, the operational models and the ICT topology are subject to the optimization of the operational concept.

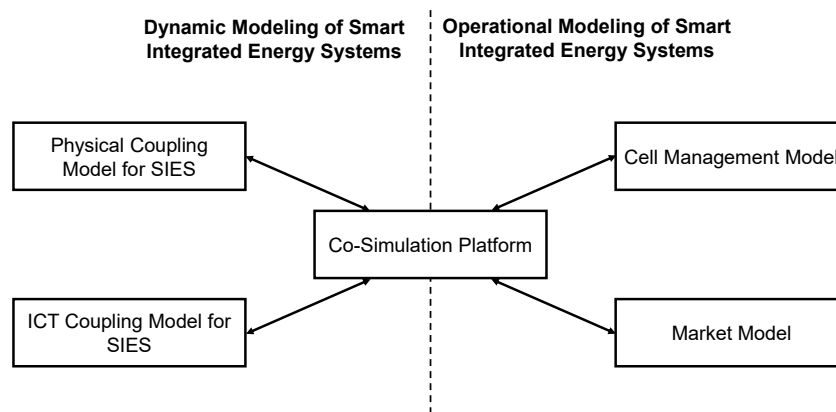


Figure 6. Simulation concept.

4. Findings

In this chapter, the first steps towards the validation of the concept are presented. Since energy system scenarios as well as the criteria for evaluation form the basis for the concept, these were developed first and are presented in this chapter. In addition, Section 4.2 deals first with the concepts of co-simulation of the models forming the SIES, but also with the realization of a proof of concept.

4.1. Energy System Scenarios 2050

With the aim of modeling future energy systems, profound assumptions for technical, economical and political features have to be made. The influence of the three aspects on the operational concept for the SIES is crucial, while the prediction of future energy system architectures is difficult at the same time. Expert statements and studies from different parties build the basis for these assumptions. To handle uncertainties, it is common to derive scenarios which cover the different possible future developments. Two basic scenarios (scenarios A and B) are compiled in the following. For this, three different sources (1 to 3) are employed, which all point out different possible pathways for the development of the energy system under different assumptions and objects of consideration. A progressed energy transition, digitization in distribution grids and a fully regenerative energy supply are prerequisites for the choice of studies and scenarios, as these aspects are the core of the system to be studied.

ENTSO-E and ENTSOG set up expert questionnaires in order to show up two major possible pathways for utilizing infrastructure for electricity and gas [52]. Two scenarios were built, each having the Paris Agreement and greenhouse gas (GHG) reduction targets as their aims. The first one, Global Ambition (1.A), assumes a wide distribution of different, mostly centralized technologies with global energy flows. Imported derived fuels such as methane and liquid e-fuels and technologies such as nuclear and CCS support the decarbonization progress. For this, a fast and global transition to green technologies is required. The second one, Distributed Energy (1.B), requires a high approval of the society for renewable energies and energy efficiency, leading to a higher local energy autonomy. Decentralized technologies, e.g., heat pumps, PV and wind, are widely in place [52].

The use of sustainable technologies is decisive for climate targets. In order to obtain a second view, scenarios from a study conducted in Germany [53] are combined with the scenarios from ENTSO-E and ENTSOG. Scenarios were derived on the basis of opinions from experts and evaluated using the story-to-simulation approach. Hereby, the qualitative opinions and assumptions were transformed into quantitative decision alternatives. Two scenarios, both reaching climate targets, are compatible with our projects goals. The main difference regards the acceptance and support of the population. In scenario one (2.A), the population resists, leading to more centralized technologies. Industry benefits from digitized distribution grids, but consumers are more inflexible in demand and supply. In scenario two (2.B), energy transition is supported widely. The efficient utilization of DERs leads to a lower energy intensity and local cross-sectoral energy flows [53].

Digitization assumes a central function within the SIES and is the basis for reaching the climate targets efficiently. A study conducted by the German Academy of Science and Technology (acatech) explores the possible scenarios within the energy system by 2030 depending on the degree of established digitization [28]. The scenarios “Complexity trap” (3.A) and “sustainable and economic” (3.B) achieve the climate objectives and are thus combined with the ENTSO-E and NEDS scenarios, in order to analyze the digitization aspect within the SIES. Scenarios 3.A and 3.B differ on two points, the homogenization of the ICT infrastructure and the standardization of IT solutions. Scenario 3.A is characterized by the establishment of a heterogeneous ICT infrastructure due to an inconsistency of economic and political actors. This leads to a low affluence of consumer flexibility solutions, resulting in a low acceptance among the population. In scenario 3.B, a homogeneous ICT infrastructure named as plug and play leads to a standardization of IT solutions but also to a spread of consumer flexibility techniques, resulting in a high acceptance among the population [28].

The scenarios and corresponding key factors are merged in order to obtain a more comprehensive view and to build a framework for technology assumptions. Many key factors coincide, mainly the support of the population for the energy transition, the application of local technologies for energy supply and the flexibility of energy consumption. Scenarios 1.A, 2.A and 3.A are in line, as well as scenarios 1.B, 2.B and 3.B. Based on the sources, a list of key factors for scenario definition was compiled, which can be found in the appendix in Table 1. In coherence with these basic scenarios, additional aspects have been included regarding market structures. Accordingly, a scenario that is characterized by the widespread acceptance of the system and its technologies (scenario B), features a higher cost advantage for renewable energy sources due to a more efficient use in contrast to a centralized system, which relies more on different energy carriers and thus has a higher cost efficiency for reserve power plants (scenario A) [54]. In line with the respective degree of acceptance, scenario B is characterized by a stronger focus on sustainability and the local energy supply in both, market behavior and in the objectives of the market mechanisms and pricing schemes, than scenario A, which prioritizes cost efficiency and profit maximization. A comprehensive overview of the scenarios is presented in Table 1.

Table 1. Technical, economical and political features for scenario generation.

Features	Characteristics	Scenario A	Scenario B		
Technical Features	Power generation structure	1. Local small-scale production (private) 2. Distributed renewable generation (commercial)	1: Low 2: High	1: High 2: High	
	Heat supply	1. Electric heat pumps 2. Hybrid heat pumps 3. District heating	1: Medium (~45%) 2: Low (~20%) 3: Medium (~35%)	1: High (~70%) 2: Low (~10%) 3: Low (~20%)	
	Energy management	1. Centralized energy management 2. Dezentralized energy management	1: High 2: Low	1: Low 2: High	
	Energy mix/primary energy sources	1. PV 2. Wind 3. Bio-energy	1: High 2: High 3: Low	1: High 2: Medium 3: Low	
	Reserve power plant	1. CHP 2. Gas turbines (methane, hydrogen) 3. Battery storages	1: Medium 2: Medium 3: Low	1: Medium 2: Low 3: Medium	
	Focus of consumption	1. Convenience 2. Sustainable consumption	1: High 2: Low	1: Medium 2: High	
	Acceptance	1. Resistance 2. Support	1: High 2: Low	1: Low 2: High	
	Grid digitization	1. Complete digitization	1	1	
	Technical requirements for the CA	1. Full compliance	1	1	
	Mobility (private, public transportation)	1. Battery electric cars 2. Fuel cell cars 3. Combustion cars	1: High (~75%) 2: Low (~15%) 3: Low (~10%)	1: High (~90%) 2: Low (~5%) 3: Low (~5%)	
	Mobility (freight traffic)	1. Electric 2. Fuel cell 3. Combustion	1: Low (~10%) 2: Medium (~30%) 3: High (~60%)	1: Medium (~20%) 2: Medium (~25%) 3: High (~55%)	
	Flexibility options	1. Batteries (home-/quarter storage) 2. Price control 3. Electrolyzers (hydrogen)	1: Low to medium 2: Low 3: High	1: High 2: Medium 3: Low to medium	
	ICT Features	Interoperability/standardization of ICT	1. Stand-alone solution 2. Plug and play infrastructure	1	2
		New services and products	1. Basic services 2. Killer apps	1	2
		Communication technology	1. B-PLC (last mile) + LTE/FO (cell manager) 2. 5G/450 MHz/FO	1	2
Market Features	Local market participation	1. Private 2. Commercial	1: No 2: Yes	1: Yes 2: Yes	
	Objective priorities	1. Economic efficiency 2. Ecological sustainability	1: High 2: Low	1: Medium 2: Medium	
	Pricing scheme	1. Economic merit-order principle 2. Multi-criteria pricing algorithms	1: Yes 2: No	1: No 2: Yes	
	Power generating costs	1. Renewable sources 2. Reserve power plants	1: Medium 2: Medium	1: Low 2: High	

4.2. Simulation

In order to examine the expected future architecture of the energy system, a concept of the SIES model has been prepared, which includes the physical system model, the ICT model, the market model and the cell management model. The physical system is modeled

with the Modelica programming language due to the TransiEnt library, an open source software for coupled energy networks. OMNeT++ has been chosen for the modeling of the ICT System because it has ready-to-use components for many application areas such as the INET library. The market and cell management model are implemented with Python due to its high-level tools and easy to use syntax. To link these four models, a co-simulation is necessary to ensure the exchange of information and the time synchronization. For this purpose, two co-simulation methods are presented.

The first method consists in using Mosaik as a co-simulation platform implemented in Python. Equipped with its own simulation clock, Mosaik allows the synchronization of the different models. Its direct connections with the different models enable it to ensure the exchange of information. Since data exchange with the physical model on Modelica requires the use of Functional Mock-up Units (FMU), FMI (Functional Mock-up Interface) is chosen to allow data exchange between the Mosaik co-simulation platform and the physical model due to its simplicity of integration, but also for the speed of communication it provides. Since the market model and the cell management model are implemented in Python, their integration with Mosaik is easy to achieve. To connect the ICT model to the co-simulation platform, a socket-based connection is established. Given the presence of a simulation clock in OMNeT++, a synchronization mechanism is needed to coordinate the two simulation clocks, one on Mosaik and the other one on OMNeT++. Since the ICT model is responsible for the data transfer, synchronization is necessary at each communication between the two models, which makes this approach costly and time-consuming.

Since the data transfer between the different models and communication modeling are two interdependent tasks, in the second approach, OMNeT++ is proposed as an ICT model simulator in the C++ programming language, but also as a co-simulation platform. The presence of a C-implementation of the FMI-Client allows an easy integration of the physical model on Modelica within OMNeT++. Unlike the first approach, the presence of an ICT model within the co-simulation platform does not require the implementation of a synchronization mechanism. The integration of the market and cell management models implemented on Python into OMNeT++ through a communication socket allows for data exchange between both instances. In this case, both instances are not time-synchronized due to the presence of the two models in two different processes. An alternative to this is the use of Omnetpy, an extension allowing one to write OMNeT++ modules in Python. This allows the merging of the market and cell management models on one side and the co-simulation platform on the other side into a single process without an additional synchronization mechanism.

The second method has been chosen to realize a proof of concept of the SIES model. The connection between OMNeT++ and the physical model on Modelica has been implemented. The architecture presented in Figure 7 allows the regulation and control of solar power plant models implemented on Modelica from OMNeT++. The control unit regulates the physical model by sending global radiation values to the proxy module which, in turn, encapsulates the message in an FMI-client compliant message format. The Proxy is an application-specific module and thus enables a clear separation from the FMI-client. In turn, the FMI-client sends the required radiation variable to the physical model, lets the FMU simulate for a specified time period and then reads other variables such as active power, grid voltage and grid frequency.

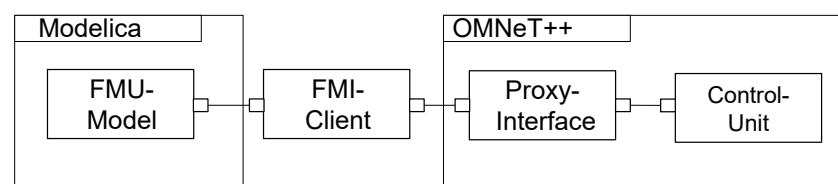


Figure 7. Architecture for co-simulation of OMNeT++ and Modelica.

4.3. Evaluation Criteria

In order to assess the simulated system’s compliance with the overall objectives of ecological sustainability, resilience and economic efficiency, evaluation criteria were defined a priori. Table 2 provides an overview of the criteria, which were chosen on the basis of [43,53,55,56].

Table 2. Evaluation criteria.

Ecological Sustainability	Resilience	Economic Efficiency
<ul style="list-style-type: none"> Greenhouse gas emissions Organic and non-organic compounds Total grid efficiency Share of renewable energies Utilization rate of renewable plants Total greenhouse gas emissions 	<ul style="list-style-type: none"> Cumulative hours lost for customers Cumulative hours lost for critical infrastructure services Resilience index for energy supply to customers Resilience index for energy supply to critical infrastructure services 	<ul style="list-style-type: none"> Energy price for consumers Energy price for producers Flexibility costs for cell managers Operating costs for energy transport and conversion Levelized cost of energy

Performing a multi-criteria energy system evaluation requires a systematic method to develop an overall indicator on the basis of a variety of specific indicators with different units and complex interdependencies [55]. The weighted sum method [57] is an easily applicable and widely used approach and will be employed to aggregate the multiple evaluation criteria into individual indicators for sustainability, resilience and economic efficiency, respectively. In contrast to a single composite indicator, this enables a more differentiated consideration of the associated overall objectives of systems within the respective scenarios. Hence, it can be deduced to which degree the system objectives are already fulfilled and which (if any) of the objectives still need to be improved. Based on the evaluation results, adequate adaptations of system processes or parameters are carried out iteratively to achieve an overall improvement of the system. Sensitivity analyses regarding such adaptations and their impacts on the three target indicators will provide the means for defining adequate improvement measures [58].

5. Conclusions and Outlook

In this section, the main findings and contributions of this work are summarized and put into perspective, taking into account current research gaps and future research.

5.1. Conclusions

In this work, we present a concept regarding the holistic simulation and operational optimization of an SIES. Upon extracting key features and characteristics of future energy systems for the reference year 2050, two defined scenarios provide the necessary specifications for the respective simulation architecture. An iterative methodological process of performing the simulation, evaluating the results with regard to a range of predefined criteria covering the overall system objectives of resilience, ecological sustainability and economic efficiency, and implementing system adjustments in line with the evaluation results facilitates the operational optimization in a structured manner. The focal point of this process is the holistic simulation, which integrates the dynamic physical energy system and ICT models with the operational cell management and market models by co-simulation. First steps towards the realization of the concept are conducted by specifying the scenarios and evaluation criteria and implementing the co-simulation architecture.

5.2. Outlook

Future work in this project will deal with the implementation of the simulation and the application of the methodology. Different parts of the simulated SIES are in the scope

of possible optimization measures. The topology of the physical coupling model is not subject to optimization and is defined by two basic scenarios. Accordingly, the focus of this project's future work lies upon identifying insights into the optimal structure and operation of SIES's ICT, cell management and markets. The impact of the underlying processes, algorithms and parameters on the evaluation criteria will be analyzed within the scope of the design possibilities given by the respective scenarios. Ultimately, this work aims to pave the road towards creating digitized and renewable energy systems by presenting an approach for optimizing SIES and, additionally, drawing first conclusions and thereby verifying the approach. By implementing such a holistic and multi-objective SIES, a research gap is filled and further research, building upon this approach, is enabled. A validation will be conducted by implementation in lab environments in order to assess the applicability of the models to realistic use cases.

Author Contributions: Conceptualization, all; methodology, K.H., T.S., B.W., A.Y.; investigation, all; resources, K.H., T.S., B.W., A.Y., D.B., M.V.; writing—original draft preparation, K.H., T.S., B.W., A.Y.; writing—review and editing & supervision, D.B., M.V., C.B., K.F., V.T.; visualization, K.H., T.S., B.W., A.Y.; project administration & funding acquisition, C.B., K.F., V.T. All authors have read and agreed to the published version of the manuscript.

Funding: This project is financed within the I3 programme of the TUHH and the Hamburg Ministry for Science, Research, Equality and Districts (BWFGB).

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

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