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Technical report on the flexibility potentials and solutions of buildings, districts, transport, and energy-intensive industries

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1. Introduction

The future German energy supply is expected to rely primarily or entirely on renewable resources. The main challenge such an energy system would entail is the highly fluctuating nature of electrical energy from wind and solar photovoltaic (PV) power plants, with large diurnal and seasonal fluctuations. In all strategies for balancing supply and demand, the direct use of electricity without intermediate storage or conversion should be prioritized, as it tends to have a cost-reducing and efficiency-increasing effect.[1] Assuming inflexible demand negative residual loads in the order of 4000–5000 h per year are expected. Still, domestic renewable electricity generation will not cover demand during significant portions of the year. Hence, electricity importing, national and international grid expansion, energy storage, cross-sectoral integration, and flexibility options will be crucial. Green hydrogen is envisioned to play a key role as an energy carrier that can bridge different sectors and enable the temporal decoupling of energy generation and use.

To estimate flexibility potentials and develop innovative flexibility solutions in the form of concepts, methods, and software, the Helmholtz Energy Systems Design (ESD) program focuses on buildings, districts, industry, and transport. The present report provides a retrospective overview of these activities until the year 2023 by summarizing key related work and publications.

Chapter 2 is dedicated to green hydrogen as a future energy carrier that will allow the storage of huge amounts of renewable energy over different time scales and make this energy available to different sectors, most notably heavy industry, transport, and heating. Specifically, power-to-gas processes are discussed as a key technology for gaining more flexibility.

Chapter 3 reports on hybrid electrical–thermal energy storage as a flexibility option via the example of a real-world laboratory power plant. Here, waste heat is used to increase the overall efficiency of a combined large-scale battery and thermal storage system.

Chapter 4 covers flexibility potentials and solutions for the processing and manufacturing industries, which, as large energy consumers, can offer a considerable demand response if they can adapt their production in response to fluctuating electricity availability and price. Specifically, solutions based on scheduling optimization account for temporal interdependencies amongst process tasks, process material and energy flows, as well as local energy supply systems.

Chapter 5 is dedicated to sustainable energy supply for the residential sector. Focusing on building and district energy systems, the flexibility potential of these decentralized energy systems, consisting of various prosumer technologies, is quantified, thereby facilitating efficient planning and operational management. Furthermore, the increasing integration of the electricity, heat, and transport sectors on the decentralized level is addressed.

Chapter 6 presents an outline of how decentralized flexibilities can be created by integrating battery–electric vehicles (BEVs) and fuel cell–electric vehicles (FCEVs) into the electricity system. The controlled charging of BEVs could relieve the distribution grids and exploit load shifting opportunities, whereas distributed FCEVs could serve as decentralized backup power plants.

2. Hydrogen as a flexibility option

In addition to electricity as a primary energy carrier for sectoral integration, an energy carrier with a better storage capability and feasibility for use in different sectors of the energy system is necessary. Hydrogen fulfills these requirements. It can be generated from electricity, has suitable storage capabilities, and can be efficiently re-converted into electricity or other fuels. Furthermore, the existing natural gas infrastructure (currently consisting of 47 natural gas storage facilities with a total capacity of 269 TWh[2] plus the natural gas grid with a storage capacity of 130 TWh) can be repurposed for the transport and storage of hydrogen in the future. In the case of a complete substitution of natural gas by hydrogen, this storage capacity would correspond to around 120 TWh without systemic adjustments (e.g., of the pressure level) due to the lower energy density.

The various hydrogen technologies, processes and modes of operation play a crucial role as sector integration interfaces and transfer points, forming the basis for creating the necessary flexibility, contributing to the realization of comprehensive defossilization, and also enabling efficiency increases in the future energy system.[3, 4] An integral component of a hydrogen infrastructure for sectoral integration is the generation of hydrogen by electrolyzers and the usage of compressors, which will act as electrical consumers and offer additional flexibility in the supply-dependent use of electrical energy. Electrolyzers can be used at locations with different boundary conditions and output sizes. In addition to continuous operation, partial load operation is also possible in the context of load management and grid stabilization. When choosing a strategically- and economically-sensible installation site (e.g., close to large consumers, storage facilities, or critical electricity grid points), the secondary sector integration-specific function of the electrolyzers is crucial for the provision of control power, in addition to the hydrogen production aspect. Depending on the quality and diversity of the locally-available renewable energy resources on the one hand, and the integration into a large-scale and well-developed electricity transmission grid on the other, these site-specific factors result in utilization of the electrolyzers at about 2000–6000 full load hours per year in the case of hydrogen production.[5]

Independent of the range of services targeted, the use of the thermal energy generated, in parallel with electrolysis, increases efficiency. In this respect, decentralized distribution approaches significantly increase the opportunity to connect them to local heat demand, for example via a district heating network. Conversely, decentralized power plants can flexibly provide residual loads and control power from seasonally-produced hydrogen and convert it back into electricity. Fuel cells as electrochemical converters achieve the highest electrical efficiencies in this regard. The use of the resulting waste heat increases efficiency and thus reduces costs. The principle of combined heat and power generation, in conjunction with thermal storage units, has already been technically realized down to power classes of a few hundred watts. If the thermal storage units are equipped with additional electrical heating systems, control power can be offered depending on the requirements and consideration of sensible power classes. This applies equally to electrical and gas-powered heat pump systems. The potential of decentralized locations in the building sector has not yet been fully exploited. The building envelope and technical components are predestined for the generation of electricity and heat or for the storage of thermal energy.

2.1 Hydrogen infrastructure for cross-sectoral integration

Studies of power output sacrificed by curtailing wind turbines in northwestern Germany and assessments of the necessary energy storage system options conducted as part of the ENERA research project highlighted that a net amount of over 235% of local energy demand in northwestern Germany already comes from renewable sources, which occasionally requires wind turbine output to be drastically reduced (Figure 1). The power output lost with this high level of renewable energy generation (primarily wind and solar energy) would have to be stored for several months in the future in order to offset the lower amount of renewable energy being converted in weather conditions that have an impact on operation (e.g., the cold, dark doldrums).[6]

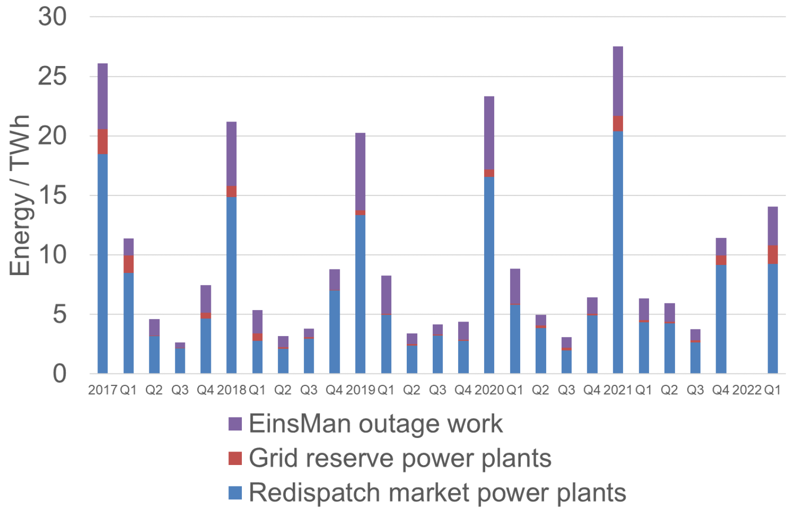

Figure 1. Network congestion management measures for the years 2017–2022 (adapted from Bundesnetzagentur).[7]

2.1.1 Hydrogen storage

Taking advantage of the synergies and interaction of the different sectors, the flexible production of large quantities of hydrogen can become a key element of the energy transition. However, large storage capacities would be required to cover the seasonal demand all year round – for example to cover the heating period or bridge a so-called "dark doldrums" (longer phases of reduced wind and solar power generation) period. Considering the current state of the art, these large storage capacities could be primarily realized by means of underground storage facilities in Germany (cavern storage in salt domes), as this type of cavern is capable of storing large quantities of hydrogen at relatively low specific costs. However, the cost advantage of this storage is countered by the disadvantage of limited regional presence in the entire country. In Germany, the required salt caverns are largely located in the north of the country.[8] Thus, for the supply of hydrogen to other regions, either a more expensive decentralized infrastructure or the interregional transport of hydrogen will be required.

As noted above, one option for the chemical storage of large quantities of renewable energy involves converting it into hydrogen and storing it in salt caverns. Hydrogen poses different technical challenges compared to fossil fuels on account of its volatility. It must be pure enough to be used to generate electricity further down the line with the help of fuel cells, meaning that potential contamination processes caused by its storage in caverns must be investigated. In particular, related research questions concerning the storage of hydrogen for subsequent use to produce electricity in combined heat and power (CHP) plants and fuel cell vehicles are being studied as part of the HyCavMobil project and are presented in this section. The infrastructure required for measuring hydrogen gas purity was also designed and constructed in accordance with the DLR activities.[9]

Measuring hydrogen purity is a difficult task, as the requirements from the ISO standard 14687:2019 (equivalent to DIN EN 17124) range into the parts per billion (ppb) scale for some of the defined impurities, especially the highly reactive sulfur components. These lead to a permanent reaction with the platinum catalyst and therefore to permanent damage to the fuel cell system. The main analysis system is based on a combined electron impact mass spectrometer (EI–MS) with an ion-molecule reaction mass spectrometer (IMR–MS). Thereby, the low limits of detection required can be achieved in a single device for almost all of the impurities defined in the standards.

This research directly contributes to an interdisciplinary DLR project called HyTaZer (Hydrogen Tank Zertifizierung), for which new cryogenic and pressurized gas tanks are built and tested for different scenarios in airborne and maritime applications. The fabrication processes and types of materials used can also have a direct effect not only on ageing and mechanical failure but also on hydrogen quality and merit further research in the future.

In addition, as part of the material and hydrogen purity research initiatives, different groups at the DLR have more closely investigated electricity grids at and around cavern sites for their suitability for the future installation of electrolyzers. To fill the caverns throughout the year, large capacities for renewable power production are needed. Therefore, investigations have focused on identifying the best positions or overlap of renewable power generation, grid capacity, and cavern sites. The developed power factory model thus enables the DLR to address the question for the whole of Germany. Portions of the results are reported in the review article on the production of hydrogen from renewables and its storage in salt caverns, where economic aspects are also evaluated.[10]

Even more important than the electricity grid infrastructure is the gas infrastructure at and around the caverns. The feasibility and demonstration of large-volume underground storage facilities for hydrogen has been undertaken for the projects H_2Cast-Ready and Prove. Therefore, the aim of the projects is to prepare and test the hydrogen storage operation. For these projects, the DLR is investigating the system integration of the storage facility, as well as the aboveground plants such as, for example, the compressor stations and cleaning units in a future hydrogen infrastructure. Therefore, the DLR is conducting a dynamic simulation-based approach combined with real measured data and boundary conditions provided by the project partner.

For example, *Bekebrok et al.* analyzed the boundary conditions for compressor systems in terms of the underground storage of green hydrogen. The results of this study indicate that due to the use of green hydrogen, a larger share of storage with a duration shorter than a year can be expected in relation to natural gas. In the analyzed case, the number of storage cycles was doubled.[11, 12]

At the Forschungszentrum Jülich (FZJ), a hydrogen-based infrastructure is under development within the scope of the Living Lab Energy Campus (LLEC) initiative.[13] The main aim of establishing the LLEC testbed is to demonstrate and evaluate monitoring and control algorithms for district energy systems, which are primarily supplied by volatile renewable energy sources by means of direct use and storage. So-called energy demonstrators for the generation, conversion, and storage of renewable energy technologies are being added to the existing energy infrastructure of the FZJ. The hydrogen-based energy demonstrators comprise an electrolyzer, compressor, pipeline, pressure tank, a liquid organic hydrogen carrier (LOHC)-one-reactor,[14] and a hydrogen-based internal combustion engine. For renewable energy supply, multiple PV systems are installed. In addition to the hydrogen storage capacities, two battery energy storage systems (BESS) will serve as short-term (daily) energy storage solutions. The pressure in the pipelines and hydrogen pressure tanks are variable, which enables them to be operated at a combined storage volume. After commissioning all of the components, the hybrid energy storage system will serve as a testbed to test, e.g., model-based planning, scheduling, and control algorithms under real conditions.

In *Holtwerth et al.*[15], the operation of a hydrogen-based campus energy system is optimized while fulfilling an electricity demand and being coupled to the electrical grid. The main objective is to minimize the electricity drawn from the grid in order to reduce costs and relieve it. As well as considering perfect forecasts, the influence of real-world forecasts and measurements for weather and electrical demand is examined in detail. In *Holtwerth et al.,*[16] time series aggregation is applied to reduce computational complexity over long time horizons.

2.1.2 Hydrogen gas grid infrastructure

Both the conversion of the existing natural gas infrastructure and the construction of a new hydrogen transport one could be approaches for hydrogen transport that connect production, storage and demand. The decision as to which of the two options is more economically-attractive or better to implement also depends on the purity of the hydrogen required for the specific application. For example, storage facilities that were previously used for natural gas could release impurities and contaminate the stored hydrogen. This would not be a problem for steel production but would be for the transport sector, where high-purity hydrogen is required. As the sampling of hydrogen in general is highly challenging when these very low levels of impurities are allowed, we developed a methodology for cross-contamination-free sampling at public refueling stations at 700 bar by using a type 4 (a carbon fiber-reinforced composite with a polymer liner) vehicle tank. This technique further enables the vehicle-independent sampling of hydrogen, as an extra device is used. Other sampling systems always require a vehicle with an empty tank.[9]

The initial results show that typical contaminants acquired at refueling stations are nitrogen and oxygen, which often stems from the gas purging processes during refilling at the refueling stations when using trailer-based systems. Otherwise, contaminations could be found in the compressor systems but typically with low levels still within the permitted range of the standards. Further research is necessary on the sampling different stations and especially electrolyzers and production processes, as well as the distribution systems when it comes to pipeline transport.

Figure 2. DLR's refueling module consisting of a type 4 hydrogen tank that is used in research projects to determine the hydrogen quality at refueling stations. Quelle: DLR

For Germany, the construction of hydrogen transport pipelines is still in the early planning phase. One initial consideration by *Gils et al.* from the DLR focused on a cost-optimized approach that focused on the hydrogen exchange between federal states. They based their estimation on energy transition scenarios that are in line with the climate protection goals of the Paris Agreement and assume a predominantly national production of hydrogen.[17] According to the calculation, this pipeline infrastructure should be added or rededicated in particular to connect the center and south of Germany, and to a minor extent between the north and center of the country (Figure 3). Using these long-distance pipelines, almost a third of the hydrogen produced – corresponding to about 100 TWh of energy – would be transported. The amount of energy from the hydrogen that would be temporarily stored in underground caverns would even be slightly larger. In the same scenario, the sum of the flexibility provided by thermal and electrical storage, as well as by charging for electric transport applications, is also around 100 TWh. Only the electricity grid is an even more important flexibility option – both in terms of national exchange and imports from neighboring countries. This underlines that sector integration would be particularly effective in combination and interaction with a variety of technologies.

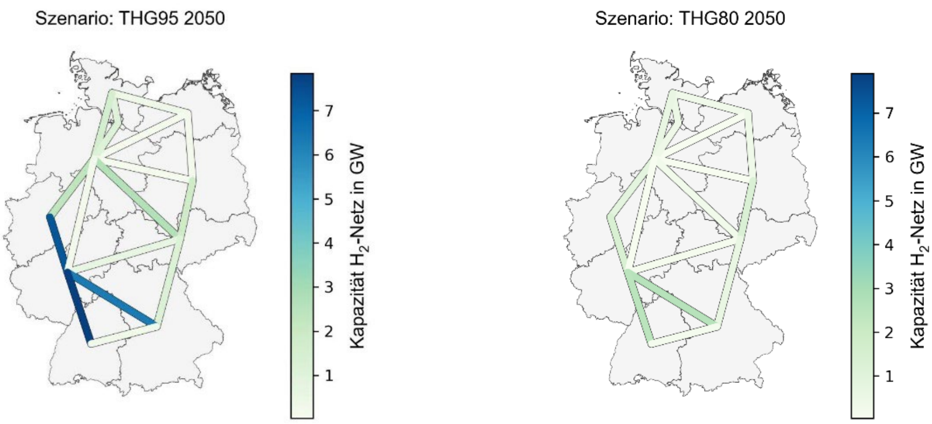

Figure 3. Expansion of the domestic German hydrogen transport network in the two scenarios (THG95/THG80) investigated in the MuSeKo project for the year 2050.

The results of the model's calculations indicates the central role that large-scale infrastructures for the production, storage, and transport of hydrogen could play in Germany's future energy system. However, the construction of such infrastructures is accompanied by major technical challenges that must still be further investigated. In addition, their economic viability strongly depends on the future cost development of the construction and use of electrolyzers, storage, and transport capacities, which is difficult to estimate today. A substantial system-analytical understanding of possible transformation pathways is therefore essential for reliable statements regarding an optimized design of the energy transition to be made.

The results described for Germany have been structurally confirmed in further DLR analyses of Australia.[18] Thereby, it has been shown that the integration of high electrolyzer capacities in combination with large underground storage facilities and hydrogen transport pipelines into the energy system can significantly reduce specific electricity supply costs. This was shown in the case of Australia using different scenarios for the export of hydrogen. Due to the higher degree of utilization of electricity generation from renewable sources, this export also brings cost benefits for domestic electricity consumers, which results from the fact that the hydrogen infrastructures required for export reduce the need for further flexibility options such as electricity storage and transmission lines. In addition, the higher utilization of the associated infrastructures also reduces hydrogen prices.

3. Large-scale battery and thermal storage as a flexibility option

In view of the fluctuating availability of renewable energy sources such as solar radiation and wind, the energy transition in the electricity sector increasingly requires the development of flexibility options. Electricity storage systems constitute an important building block for the stability of the electricity grids of the future.

Figure 4. Power plant Bremen Hastedt (incl. photomontage of the HyReks infrastructure). Quelle: swb AG

Due to the lack of possibilities for storing electrical energy on a large scale in the electricity grid, modern battery storage systems make up a central link for keeping the constantly increasing volatile generation from renewable energy sources in balance with the different consumer load profiles. The new hybrid regulating power plant in Bremen Hastedt (see Figure 4), which is being researched by the DLR, can ideally provide a frequency containment reserve (FCR) due to its fast reaction. In addition, the system is able to provide a negative FCR for the district heating supply by means of sector recoupling. This will displace the production shares of a heat-led CHP plant and thus fossil energy sources from the heat supply.

The hybrid control power plant (HyReK) has a wide range of potential applications and is expected to improve both energy efficiency and supply security. In the research project, tools for the optimal design were developed, operation management strategies were designed and tested, and individual components important to the system were tested for their interaction and functional efficiency (Figure 5). Furthermore, system and operating parameters were optimized to maximize the economic efficiency of the HyReK. In addition, an investigation of the legal framework conditions of the marketing concept was conducted and the system was further optimized for simultaneous multiple uses for the respective services. The long-term impact on energy systems and sustainability was assessed through an assessment of the ecological implications by means of a life cycle analysis[19] and technology road-mapping to capture future innovations.

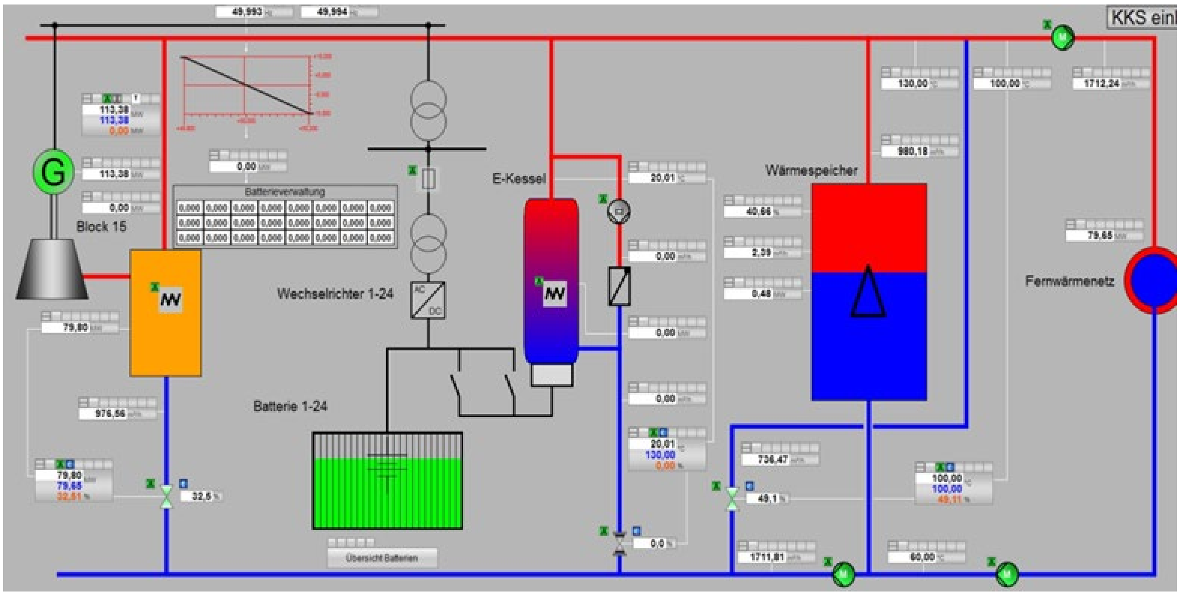

Figure 5. Functional operating diagram incorporating a battery, power-to-heat, and thermal energy storage.[20] Quelle: swb AG

The project was designed to elaborate and validate an innovative concept for the sustainable provision of primary control power.[21] Other operating options for the combination of battery storage and power-to-heat modules were also examined and evaluated within the framework of the economic and legal conditions.

3.1 Modeling the system

Technical, economic,[22] and ecological[23] models were implemented as part of the HyReK 2.0 project for the energy balance representation and simulation, as well as for the economic and ecological evaluation of the HyReK system. The technical models (Figure 6) were implemented in Python and Matlab/Simulink. In the model implementation in Python, the principal energy flows between the grid, battery, and electric boiler were mapped at an early stage together with the precise switching, recharging, and degree of freedom strategies. This operating strategy and design model were used to carry out economic and energy balance investigations. The HyReK model implemented in Matlab/Simulink was designed as a physical entity. The physical system components were programmed at a higher level of detail, as well as the individual system components at different levels of detail. At the beginning of a simulation, the model was configured on the basis of the simulation requirements, so that a balance could be struck between the level of detail and the computational effort required. During the development process, attention was paid to the interface compatibility of the model variants. All models of the physical system components can be compiled into an FMU, which can then be run in other simulation environments, including Python, for example. In fact, the physical components of the HyReK model in Python can be replaced by the FMU. In this mode, the operating strategies programmed in Python control the physically-based model. Furthermore, detailed models for the economic and ecological evaluation of the HyReK were developed. In addition to cost and material data for the different components of the HyReK system, these evaluations also include data regarding the operation of the HyReK, which was calculated using the energy balance model.[24]

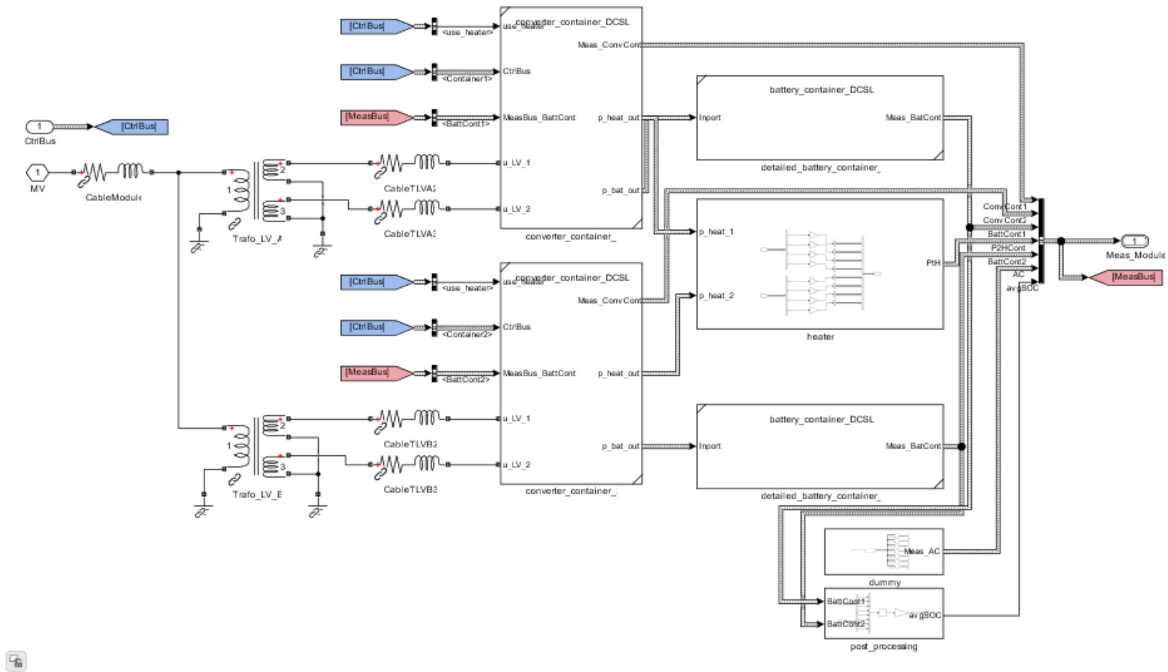

Figure 6. HyReK module as a detailed electrical model (sub-part of the overall system).[20]

Validation to real data shows a high degree of accuracy (Figure 7):

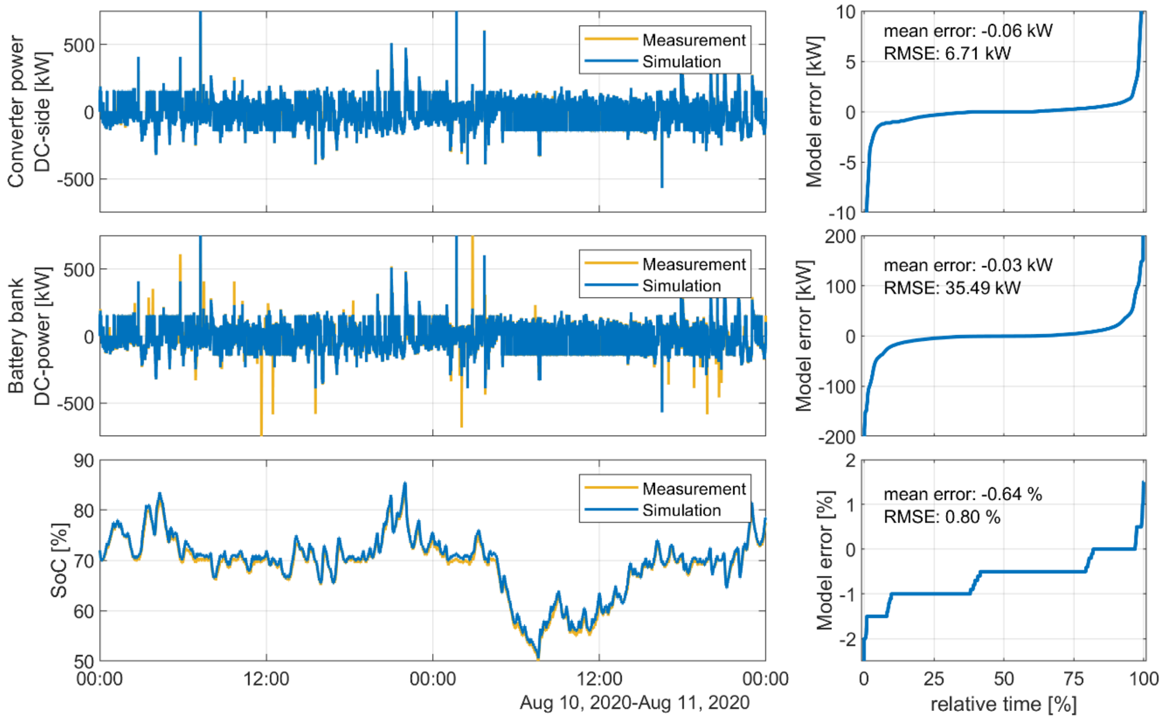

Figure 7. Simulation of one operating day.[25]

The model was used to test a variety of operational management strategies. The results of the simulations were used in an economic analysis by *Worschek et al*.[26]

3.2 Optimizing the FCR by four different applications

The impact of the battery aging due to different operational modes and conditions was investigated[27] and the model implemented in an economic analysis. These four application concepts (Figure 8) were compared with either the construction of a battery storage system for the provision of primary control power (for the operating strategy: the start-up of a plant) or the operation of the sector integration plant without the provision of primary control power (for the operating strategy: throttling the plant from operation).[28] The evaluation of the different operating concepts or the comparison with the respective reference system was carried out as in variant 1 using the net present value method.

A detailed description of the underlying methodology in connection with the results can be found in *Krupp et al.*[29] To provide 1 MW of primary control power with a hybrid system, a battery capacity of about 100 kWh is required. It makes a negligible difference as to whether the X-technology is used for a positive or negative PRL, or whether the battery storage operates as a stand-alone system. Differences in capacity are only noticeable when the additional reserve capacity for the 15-minute criterion is considered, because this is 250 kWh for a hybrid system and 500 kWh for a single battery storage one, and so a battery capacity of 350 kWh or 600 kWh is required.

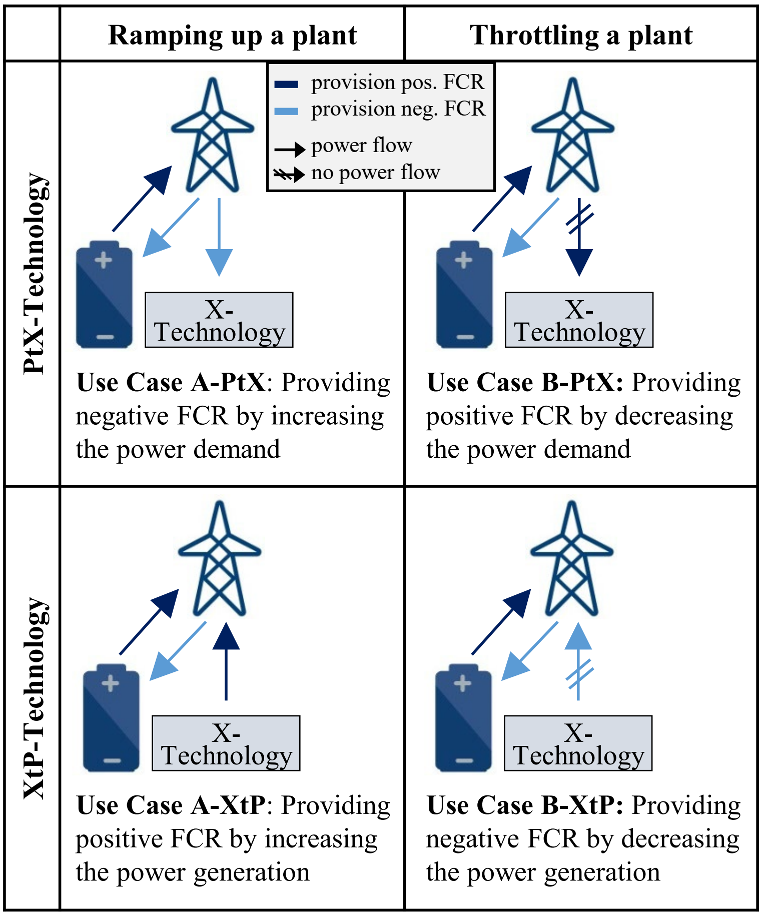

Figure 8. Comparison of the four application concepts.[20]

Based on the assumptions made regarding the annual revenues on the primary control power market (60 k€/MW p.a.) and the investment costs for a battery storage system (700 €/kWh), supplementing an existing X-technology with a battery storage system to provide primary control power always brings an economic advantage via the operating strategy of throttling a plant. In contrast, the economic benefits of building a hybrid system depend on the investment and variable costs of the X-technology used.

4. Energy-intensive industrial processes

The process and manufacturing industries are major energy consumers that can offer considerable flexibility if they can adapt production in response to varying electricity availability and prices.[30, 31] The flexibility of power-intensive production processes can be marketed on the day-ahead and intraday electricity markets, as well as on the balancing power ones.[32] Alongside improving the balancing of supply and demand in the electricity grid, demand response (DR), i.e., adaptation of the momentary production rate and thus the power draw, may offer relevant economic benefits for process operators in the form of electricity cost savings if a period of relative underproduction (at high electricity prices) can be compensated by a later period of overproduction (at low electricity prices). Determining the DR potential of a process and performing optimal DR typically requires the solving of a scheduling optimization problem that takes into account the temporal interdependencies between different process tasks and the involved material and energy flows; see, e.g., *Castro et al.*[33] and *Zhang and Grossmann*.[30] The DR of industrial systems is further complicated by the presence of the local co-generation of power and process heat and the adoption of power-to-X technologies, both of which result in the tight coupling of different energy forms. Such dependencies can be incorporated into DR optimization in the form of multi-energy system models, allowing for the integrated scheduling of the process and its local energy supply system; see, e.g., *Agha et al.*[34] and *Leenders et al*.[35] The ESD program investigates flexibility potentials and solutions for industrial energy supply systems and selected energy-intensive production processes. Mitsos (FZJ) is also a principal investigator and director of the Kopernikus project "SynErgie;" and his research group has published numerous articles on the topic, e.g., *Mitsos et al.*[31], *Brée et al.*[36], *Schäfer et al.*[37], *Burre et al.*[38], and *Caspari et al.*[39]

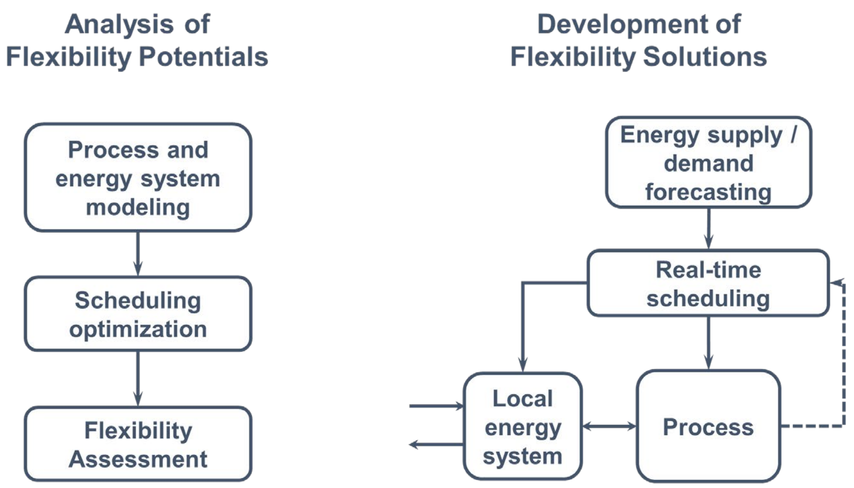

Figure 9. The FZJ and KIT use scheduling optimization to determine the flexibility potential of power-intensive production processes (left). Furthermore, they develop solutions for the real-time scheduling of flexible processes and their local energy supply systems (right).

As part of the ESD program, the FZJ and KIT focus on the development of optimization models and approaches to analyze the DR potential of industrial systems and to enable real-time DR scheduling solutions, as illustrated in Figure 9. To this end, process and energy system models are created that capture the scheduling-relevant dynamics, the relationship between production rates and energy consumption, dependencies arising from co-generation, and material and energy flows between the system components. Emphasis is placed on stochastic DR optimization as electricity price predictions are subject to uncertainty. To realize a DR scheduling that is sufficiently fast for online applications, efficient problem formulations based on reduced-order modeling and machine learning (ML) have been developed at the FZJ. Online application also requires probabilistic forecasting methods, which the FZJ develops in the form of generative ML models that can produce highly accurate time series predictions.

4.1 Analysis of flexibility potentials

With copper being a key material in renewable energy technologies, the FZJ analyzed the DR potential of copper production, a power-intensive production process that comprises continuous and batch-wise operated tasks.[40] To this end, a discrete-time resource task network (RTN) model[41] of copper production was created based on a reference plant description from the literature[42] and resulted in a mixed-integer linear program (MILP) scheduling formulation. The DR potential was assessed by first determining the maximum production volume for a two-week scheduling horizon by means of a material throughput optimization and then minimizing the electricity costs for the maximum production volume. Figure 10 shows that DR scheduling optimization based on time-varying day-ahead (DA) electricity prices shifts production to times of favorable electricity prices. In particular, electro-refining and off-gas handling from the converters are throttled or even stopped during hours of peak electricity prices. On the contrary, tasks operate at or near full capacity when electricity prices are low or even negative. The average shifted load for all 26 consecutive two-week schedules of the year 2019 amounts to 2.55 GWh.

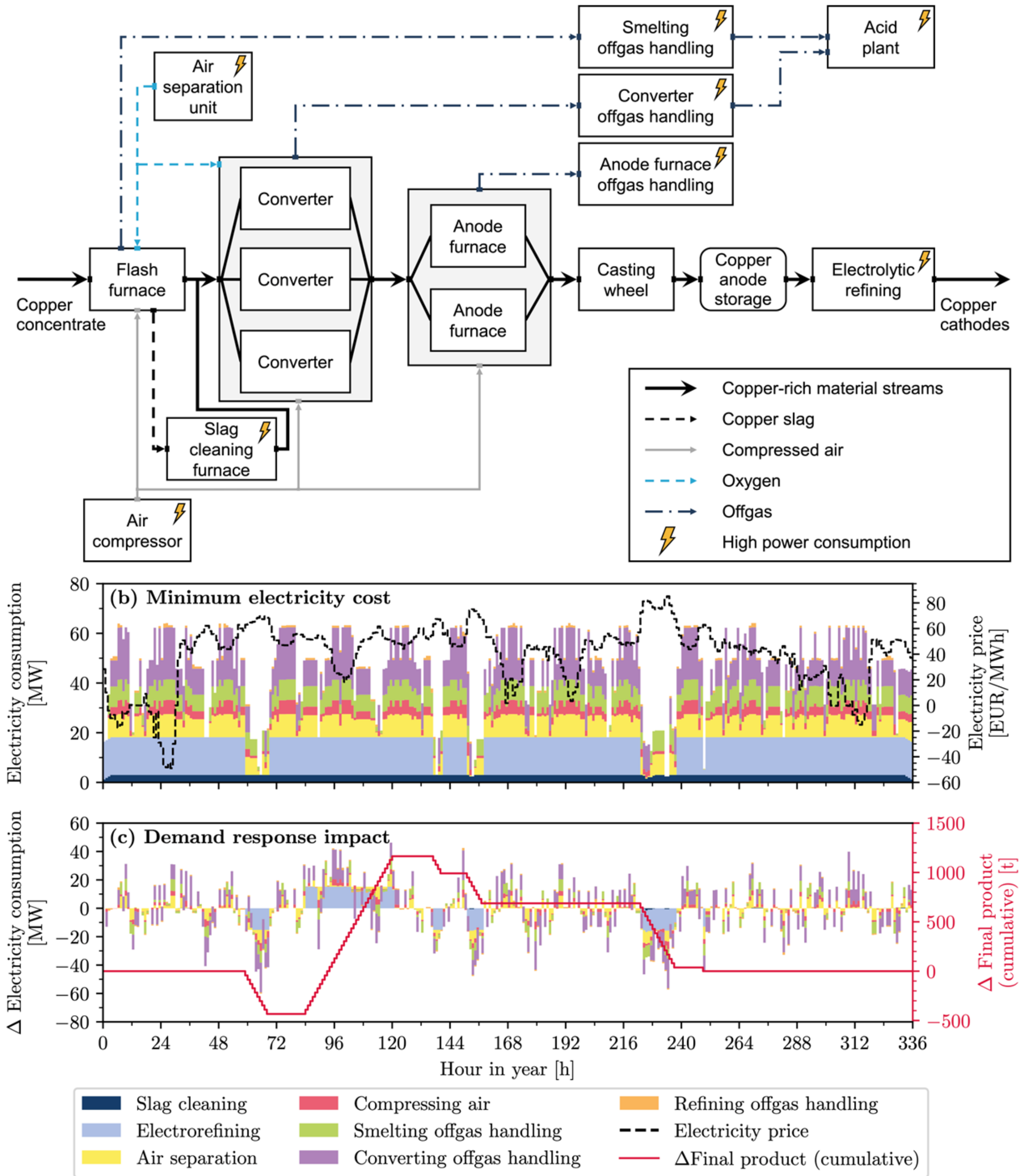

Figure 10. Demand response potential of copper production: Process flowsheet (top), optimal production schedule (center), and demand response impact (bottom) for the first two weeks of 2019. Left axis: electricity consumption; right axis: time-varying day-ahead prices (center) and cumulative change in the final product (bottom). The figure is adapted from Röben et al.[40], CC-BY-NC 4.0.

The results of *Röben et al.*[40] suggest that annual electricity cost savings of up to 14% can be achieved for copper production compared to a worst-case schedule in which power is drawn such that electricity costs become maximal. Because of the production volume constraint, the DR does not negatively affect the amount of copper produced, which is important as the value of copper vastly exceeds the cost of electricity. In a subsequent work by *Germscheid et al.*,[43] the FZJ extended the DR potential assessment to the intraday (ID) electricity market by adapting the RTN model to a stochastic optimization approach that enables simultaneous DA and ID market participation under ID price uncertainty conditions. Marketing the process flexibility in both the electricity spot markets would allow for an additional 6% in weekly savings. Furthermore, modeling the on/off decisions of the batch-wise operated tasks in conjunction with the uncertain intraday prices significantly affects the load shifting but has only a minor impact on the electricity cost savings.

As part of the Innovation Pool project, "Energy transition and circular economy" between the ESD program and the MTET one, the DLR, KIT, HZDR, and FZJ investigate the demand-side flexibility potential of the raw material industry. Due to the large heterogeneity of raw material processes, the consortium has chosen to investigate the theoretical flexibility of frequently occurring process components, e.g., smelters, mills, or dryers. The deduced quantitative parameters describing the flexibility potential of the individual components can be subsequently used to assemble process-level scheduling models, similar to the case of copper production.

As the cement industry is one of the most energy-intensive sectors in the basic materials industry, at the KIT and FZJ, cement production is being investigated to determine the extent to which demand response and demand side management can be used to achieve flexibility and grid-friendly operation. Global cement production amounts to around 3.6 billion tons per year and about 2% of the electricity generated worldwide is used for the process of grinding the raw materials.[44]. There is an electrical energy requirement of around 100–110 kWh/t of cement. The majority of the electrical energy (around 70%) is used for comminution processes such as grinding. According to *Hübner et al.*, in Germany there are 34 fully integrated cement plants and 19 plants without clinker production prior to cement grinding, which produced almost 25 million tons of cement in 2017.[45] Cement mills typically have seasonal overcapacities that offer the potential for flexibilization. Using the example of a cement plant in southern Germany, *Becker*[46] showed that optimal demand response management can achieve average annual electricity cost savings for cement mills of over 7% compared to current operation.

For continuous processes that allow for variation in the production rate by a change in power draw, e.g., chlor-alkali electrolysis with an installed capacity of 1.48 GW in Germany,[47] the FZJ used a generalized process model (GPM)[48] to investigate possible economic savings through the DR from the perspective of a process operator.[49] This work was performed as part of the Helmholtz Incubator Project "Uncertainty Quantification", as a particular focus was on optimizing the DR potential under consideration of intraday electricity price uncertainty. Parametrizing the GPM requires knowledge regarding a few important flexibility characteristics of a process that can typically be readily deduced, e.g., the available oversizing, minimum admissible part-load, ramping limitations, and efficiency losses from off-design operation. In addition to investigating the examples of chlor-alkali electrolysis, copper electrolysis, and aluminum electrolysis, the FZJ performed a parameter study analysis to determine which processes could benefit most from offering DR.[49] In particular, the economic benefit of simultaneous participation in both the DA and ID electricity markets by means of stochastic scheduling under ID price uncertainty was analyzed. The findings showed that less flexible processes can benefit comparatively strongly from marketing their flexibility on the ID market in addition to the DA market. The three electrolysis can approximately double their electricity cost savings through simultaneous market participation. Underpinning the analysis was an uninformed selection of historical ID price scenarios, suggesting that further economic potential lies in the application of more sophisticated generation of price scenarios. The developed method of combining a GPM and stochastic DR scheduling represents an early screening approach that allows for the quick first DR potential assessment of a continuous process.

4.2 Development of flexibility solutions

To leverage flexibility potential in industrial practice, real-time capable autonomous decision-making systems are required that continuously incorporate energy supply and demand forecasts, monitor the current system state, and determine optimal schedules for the operation of the process and its local multi-energy supply system. The essential building blocks and information flows underlying such an autonomous system are illustrated in Figure 11, which also displays flexibility solutions developed by the FZJ and KIT. These solutions are system technologies that take the form of tailored models, formulations, and methods.

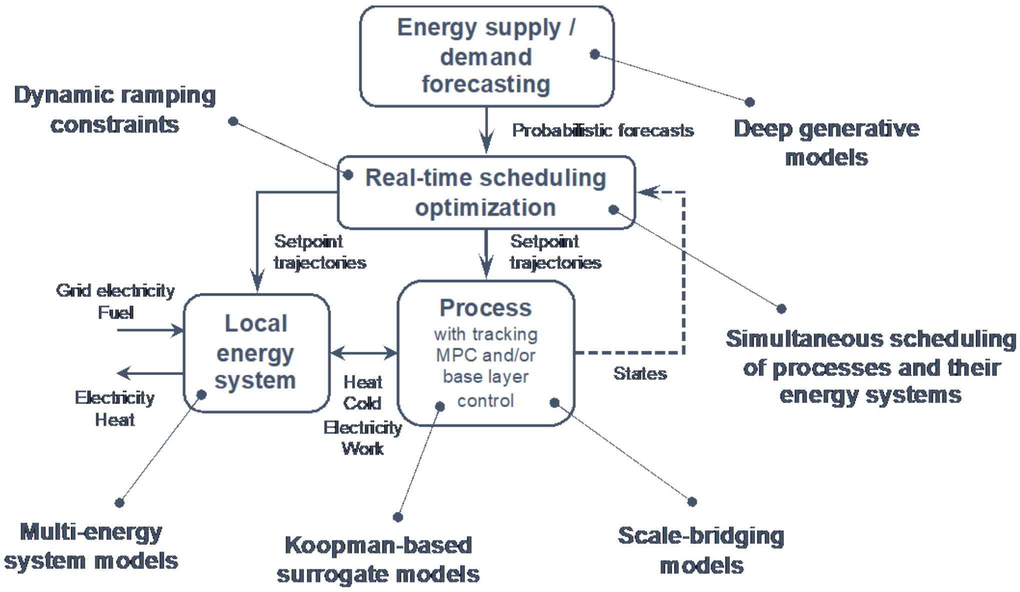

Figure 11. Flexibility solutions for the real-time scheduling of energy-intensive industrial processes and their local energy supply systems developed by the FZJ and KIT.

Computationally-efficient optimization models and approaches are essential for real-time-capable DR scheduling and the control of flexible production. Traditionally, the operations of processes and their local energy supply systems have been scheduled in a sequential fashion. Optimizing the DR capabilities of an industrial system, however, entails the simultaneous scheduling of the production and its energy system.[50] Such integrated scheduling gives rise to computationally-challenging optimization problems, as both the scheduling-relevant (nonlinear) process dynamics and the discrete on/off decisions of the energy system components must be incorporated into a single optimization problem. The FZJ developed an efficient formulation for such simultaneous scheduling based on a scale-bridging model (SBM)[51] of the closed-loop process dynamics and a piecewise linear multi-energy system model, eventually resulting in a MILP that can be tackled in computational times, allowing for online application with state-of-the-art MILP solvers.[50] The simultaneous dynamic scheduling (SDS) approach was applied to single-product and multi-product continuously stirred tank reactors (CSTRs), as well as a distillation column. In the latter case, the SDS approach leads to a 5% decrease in operating costs compared to typical steady-state operation. The resulting flexible operation for exploiting variable electricity prices is shown in Figure 12. Optimal DR scheduling causes the electric boiler to operate at high loads when electricity prices are low, whereas otherwise only the combined heat and power plants satisfy the heat demand of the column. The SDS method is transferable to other applications with relative ease, as the underlying SBM is effectively a surrogate model that can be parametrized and tuned based on process data or simulations.[50]

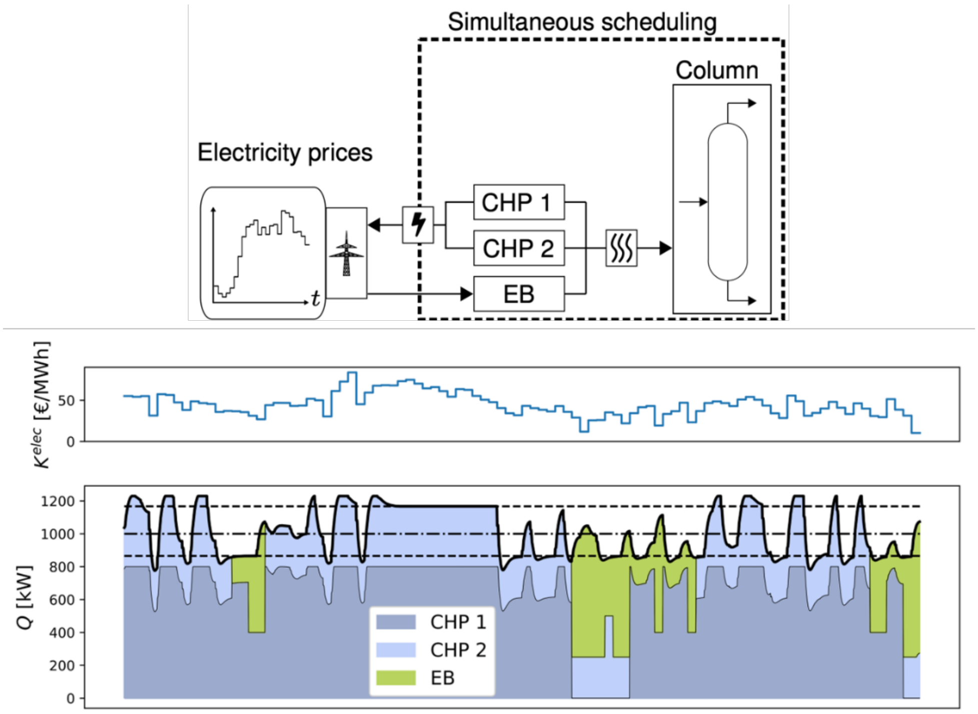

Figure 12. Simultaneous dynamic scheduling (SDS) of a distillation column and its local energy supply system consisting of two combined heat and power plants (CHP1 and CHP2) and an electric boiler (EB): In times of low electricity prices K^{elec}, the electric boiler is used to supply parts of the heating duty Q. The figure is adapted from Baader et al.[50], CC-BY 4.0.

As an efficient DR formulation for processes with high-order dynamics, the FZJ proposed the concept of dynamic ramping constraints (DRCs), i.e., constraints that, unlike standard ramping constraints, are a function of the process state.[52] The use of a piecewise linearization allowed the derivation of a MILP formulation for the simultaneous scheduling of the process and its energy system. The DRC framework was first applied to single-input, single-output (SISO) processes. An illustrative case is shown in Figure 13, where the operation of two CSTRs and their local supply system is optimized, achieving a 41% improvement in operating costs compared to steady-state production. Here, the cost-optimal schedule shifts the production of the CSTRs in time such that their waste heat can contribute to covering on-site heat demand, thereby almost completely avoiding expensive operation of an electric boiler. The FZJ recently extended the DRC approach to flat multi-input, multi-output (MIMO) processes.[53]

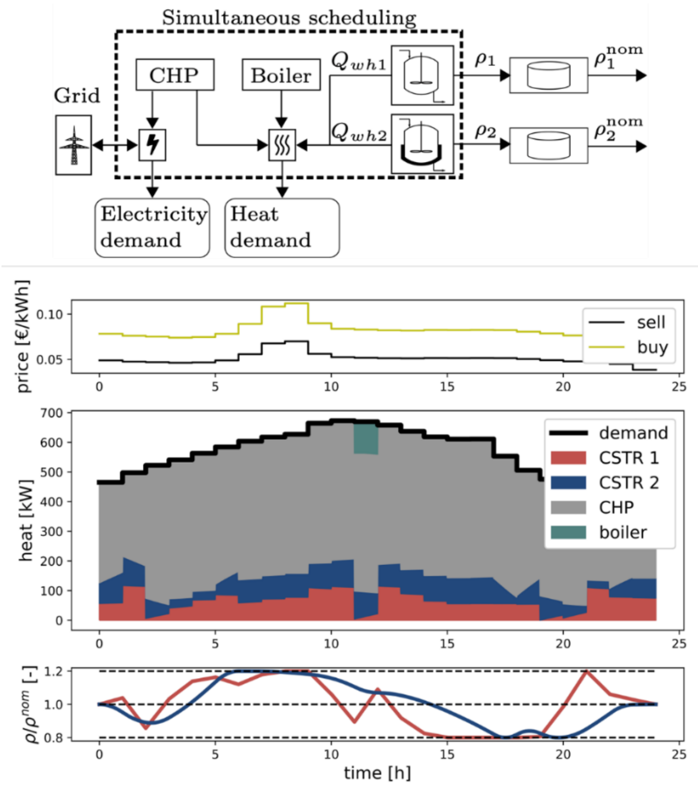

Figure 13. Dynamic ramping constraints (DRCs) for the simultaneous scheduling of two CSTRs and a multi-energy system consisting of a combined heat and power plant (CHP) and an electric boiler: The production ρ is shifted in time such that the boiler must rarely be turned on, as CSTR waste heat is used to partially cover the on-site heat demand. The figure is adapted from Baader et al.[54], copyright: Elsevier.

ML-based surrogate models, e.g., artificial neural networks (ANNs), constitute a further promising option to enable real-time-capable scheduling and nonlinear model predictive control (NMPC). The FZJ has investigated the derivation of optimal surrogate models as part of a doctoral project in the Helmholtz School of Data Science in Life, Earth, and Energy (HDS–LEE). To this end, Koopman-based surrogate models were utilized in which ANNs transform an originally nonlinear process model into a higher dimensional linear state space in which fast convex optimization techniques can be applied.[54] Surrogate models are typically trained through system identification (SI), which minimizes the mean squared error on simulation samples but does not explicitly consider the target application of the model predictive control (MPC). The FZJ recently proposed a method to fine-tune Koopman-based models initialized via SI by means of end-to-end reinforcement learning (RL) and thus create task-optimal surrogate models for use in DR optimization.[55] Applied to a CSTR, the RL-tuned surrogate model achieves a more effective and economical NMPC, i.e., higher operating cost savings compared to SI-trained surrogate models with identical architectures, while also reducing the violations of production quality constraints. RL-tuned Koopman-based surrogate models thus constitute a promising avenue towards the real-time-capable DR optimization of processes with nonlinear dynamics.

The provision of industrial flexibility typically takes place under conditions of uncertainty, especially regarding electricity prices. Obtaining accurate price forecasts that are accompanied by an uncertainty measure is therefore important, as is explicit consideration of prediction uncertainty in DR scheduling. The latter can be achieved via stochastic scheduling approaches that utilize optimization in conjunction with uncertainty techniques. As part of the Helmholtz Incubator Project, “Uncertainty Quantification”, the FZJ investigated the case of an industrial process that markets its flexibility on both the DA and ID markets.[49] In particular, uncertain ID prices were accounted for at the time of DA market commitment by a set of historical electricity price time series used as scenarios, which led to a two-stage stochastic program. In addition to the minimization of the expected value of the electricity cost, the approach can be used to minimize the financial risk of market participation under price uncertainty. As risk-averse scheduling is computationally-expensive, a heuristic sequential scheduling approach was proposed that yielded similar economic DR performance as the stochastic scheduling, but with a significant improvement in computation time.[43]

Aiming for accurate time series forecasts that are accompanied by a measure of uncertainty, the FZJ developed a fully data-driven prediction approach as part of a doctoral project at the HDS–LEE. In particular, the approach combines principal component analysis (PCA)-based dimensionality reduction with normalizing flows (NFs) – a special type of deep generative ML model that uses invertible neural networks to relate data from a target distribution, e.g., electricity price time series data, to samples from a Gaussian distribution.[56] The NF approach was applied to an illustrative wind farm operator bidding problem in which wind power generation scenarios were predicted by the NF using a deterministic wind speed forecast and subsequently utilized in stochastic scheduling.[57] Here, the NF approach outperformed other data-driven prediction approaches in terms of distribution representation, daily trends, and profits in day-ahead bidding. The FZJ also developed a multivariate probabilistic forecasting model of ID electricity prices using NFs that incorporates various external impact factors such as renewable electricity forecasts.[58] Using explainable artificial intelligence, the previously-realized ID prices and the corresponding increments of the DA prices were found to be the major external driving factors of ID prices. The novel multivariate forecasting approach yields both sharp predictions and reliable prediction intervals as a measure of prediction uncertainty (see Figure 14).

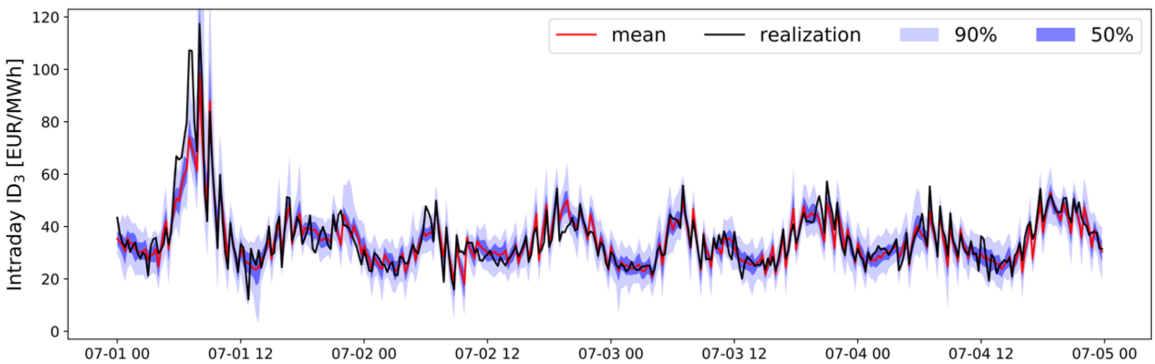

Figure 14. Probabilistic intraday price forecasting with normalizing flow (NF): The mean NF prediction (red line) is compared to the true price (black line). The blue shaded areas show the 50% and 90% prediction intervals. The figure is adapted from Cramer et al.[58], copyright: Elsevier.

The grid-friendly operation of energy-intensive processes can be achieved by adjusting production to the forecasted electricity supply and thus to electricity prices. Due to the high electricity consumption of grinding processes and the possibility of batch operation, solutions for the optimal planning and operation of mills are being researched at the KIT using the example of cement mills. Cement plants usually have several electric mills for processing cement clinker into cement with seasonal overcapacities that offer potential for flexibilization. The average electrical power per cement mill in Germany is 2.2 MW, with an average output of 40 t/h and a specific electricity consumption of around 51 kWh/t of cement.[45] In the optimal mill scheduling framework developed at the KIT, a type-specific delivery forecast for approximately one week was considered. Optimal DR is achieved by optimizing production planning based on the forecasted electricity price time series of a week. In addition, compliance with atypical grid usage can be ensured as a boundary condition in production planning, which leads to the avoidance of high consumption at peak load times during parts of the year (winter) and thus a reduction in the grid fee to be paid. The KIT formulated cost-optimal and thus grid-friendly production planning for a week with several mills, cement types and silos, considering all relevant boundary conditions, as a MILP. By updating the electricity price and supply forecast on a daily basis, production planning can react to changing boundary conditions in the electricity grid and at the consumer. Together with an industrial partner, a prototype for the optimal scheduling of cement mills was developed at the KIT and is currently being tested and validated by the partner.

The design of an industrial energy system has a significant influence on the flexibility potential. To this end, the FZJ proposed an optimal retrofit of copper production by power-to-hydrogen technology where on-site co-generation of hydrogen and oxygen allow for the exploitation of time-variable electricity prices.[59] The analysis showed that such decarbonized copper production could become a viable solution both economically and environmentally if expected improvement in the economic and technical performance of water electrolysis systems materializes, CO_2 emission certificate prices rise considerably, and a largely decarbonized electricity mix becomes available. As many industrial energy supply systems will need to be redesigned to achieve CO_2 emission targets, the possibilities for integrating flexibility options, e.g., in the form or power-to-X technologies, should be explored at the design stage. The FZJ developed the energy systems optimization framework COMANDO, which allows the design optimization of local energy supply systems to be performed, taking flexibility potentials and thus DR capabilities into account .[60] COMANDO[1] is an open-source Python package in which multi-energy systems can be described in a component-oriented manner with nonlinear, dynamic, and discrete features. In addition to its application to industrial systems, it is a core element of the tools and an ICT platform for building and district energy system optimization developed at the FZJ (cf. Section 5).

In collaboration with the Helmholtz program MTET, the KIT is researching a new process for the grid-friendly, dynamic production of green methanol. All of the necessary process steps (electrolysis, methanol synthesis, distillation, CO_2 absorption, and desorption) are being investigated in the KIT Energy Lab utilizing a container-sized test plant. A particular challenge in this context is the dynamic operation of such a plant with the aim of achieving grid-compatibility. Therefore, DR methods are being further developed and investigated prototypically for the power-to-methanol process, including the automatic or semi-automatic generation of DR models. The work will be further expanded as part of the EU Horizon Europe project, UP-TO-ME.

[1] https://jugit.fz-juelich.de/iek-10/public/optimization/comando

5. Buildings and Districts

As well as the local use of energy sources, electricity generation from renewable energy will also be organized in an increasingly decentralized way. With the exception of offshore wind turbines, most of the power stations based on renewable energy sources are located at or below the 20 kV grid level. The significant economies of scale involved in PV installations and wind turbines means that these power stations are being increasingly operated by local stakeholders who expect to derive some commercial or environmental policy benefit from their efforts.[61]

The fact that generation systems are increasingly decentrally organized means that the sector integration of electricity, heat, and transport can be the key issue regarding decarbonization, particularly at the regional level.[62] This suggests that the focus of research and development in the field of renewable energy-based energy system solutions should be at the individual property, district, and building levels. In addition to reducing CO_2 emissions, the targeted grid-serving operational management of regional energy systems can help relieve pressure on higher-level electricity grid tiers.

In order to assess the flexibility potential of decentralized energy systems consisting of various technologies, the DLR developed a technology-agnostic method for dynamic flexibility quantification.[63] This method is capable of determining the time-varying flexibility reserves of technologies whose primary application purpose is not flexibility provision but, e.g., heat generation or transport (Figure 15), and aggregate the potential of different technologies (Figure 16).

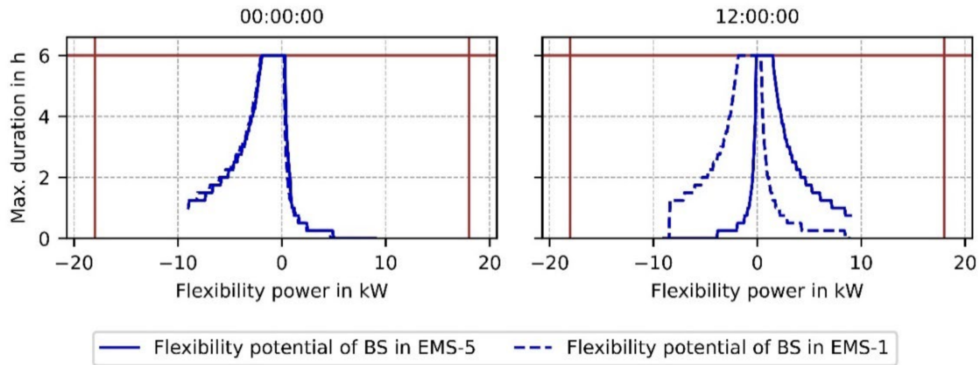

Figure 15. Flexibility potential of two components with different operating behaviors.[64]

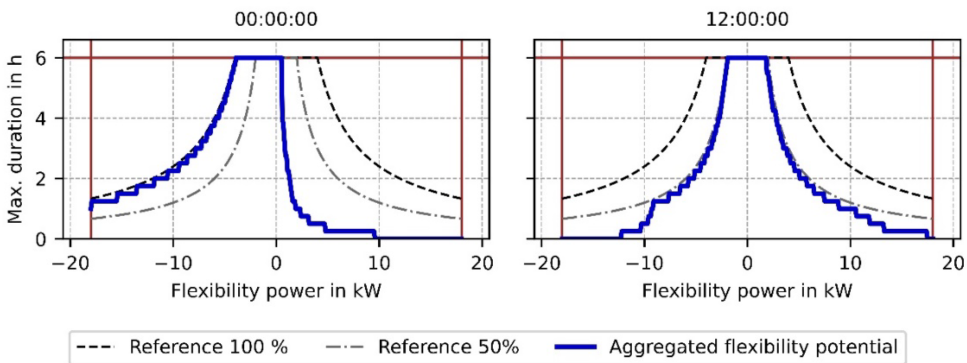

Figure 16. Aggregated flexibility potential.[64]

Therefore, methods and technologies for the efficient planning and operational management of buildings, residential neighborhoods, and urban areas are being studied at the DLR and their potential for technical and economic flexibility evaluated. Here, the focus lies on the user's point of view without consideration of the impact on system stability.

5.1 Energy components at the building level

Enormous progress has been made over the past 20 years in developing components for sustainable energy supply systems. Competitive production costs have helped electricity generation from PV installations or wind turbines develop into a driver of the energy transition. The DLR has been conducting successful research into new components and making a major contribution to the development of battery storage systems, electrolyzers, and fuel cells. However, in addition to component development, their integration is also crucial. The DLR has focused specifically on the integration of sector-integrated technologies in this context. As an illustration, the integration of heat pumps in a building system is discussed in the following section.

Heat pumps have significant potential for stably supplying heat to buildings by using electricity from renewable energy sources and thus decarbonizing room heating. With the aim of reducing the final energy consumption of existing apartment blocks by up to 80% by exploiting potential savings, the DLR collaborated with 17 European project partners from six countries on the BuildHEAT research project. The principal task of the DLR was to benchmark and validate an air-to-air heat pump system. In addition to finding an operating method that was as energy-efficient as possible, the aim was to also identify potential areas for optimization and recommend actions based on these. In this context, the heat pump system serves a heating, cooling, and ventilation function for apartments, as well as supplying hot water for domestic use. The operational management strategies had to take the use of locally-generated PV electricity into account.

Figure 17. Test bench facility for evaluating the air-to-air heat pump system at the DLR. Quelle: DLR

The climatic constraints on the future demonstration site in Zaragoza within the project BuildHEAT were mapped using test methods that the DLR had internally developed. The test facility shown in Figure 18 allows different representative air temperatures to be emulated while also acting as a heat source or sink. The heat pump (pictured on the right) can thus be realistically operated and dimensioned and, above all, reproducibly. The test methods involve daily profiles with typical temperature patterns, heat and cold loads, and radiation data. These were supplied as annual data records by a project partner (see Figure 18) and transferred to time-lapse tests at the DLR.

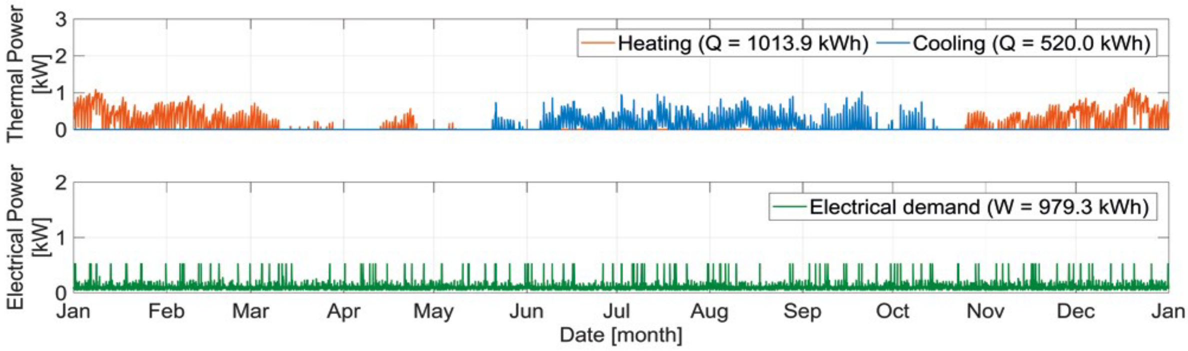

Figure 18. Visualization of the expected energy demands after renovation of the Zaragoza apartment measuring 85 m². The chart above shows the heating and cooling requirements for the heating and air-conditioning of the renovated flat at the Zaragoza demonstration site, which form the basis for reproducing the test profiles. The bottom panel displays the corresponding outside temperature, as well as the amount of solar radiation. The electrical load profiles were also validated but not considered in the tests.

To this end, actual days were classified by their climatic and energy characteristics, and their distribution and frequencies were evaluated. The methods and simulation tools developed were then used to combine representative single days into a shortened year-long cycle, resulting in reduced test times of 21 rather than 365 days. Generation and requirement profiles were specified and performance and energy KPIs calculated. The test reproduced the heat requirements of the flat on specific days, which had to be incorporated into the system. These requirements consisted of different heat and cold loads depending on the season and hot water profiles, supplemented by PV radiation profiles. Target and actual values were recorded and compared to evaluate the reproduction quality of the test design and calculation of the energy KPIs. The amount of power required by the electrical consumers in the heat pump system – primarily the compressor, additional heating rod, and fan – was also logged.

The performance rating of a heat pump indicates the ratio between the heating power it produces and the electrical power consumed by the compressor and balance of plants. Unlike the generally more or less stationary operating modes used for performance tests of this kind, the operation of the heat pump was highly dynamic in terms of its operational and temperature management. As expected, lower performance ratings were achieved as a result of the additional requirement to ventilate living spaces and prepare hot water. The value designated in the project as the "thermal energy to operating power ratio" (TOR) was 1.75, meaning that 1 kW of electrical energy is required to produce 1.75 kW of heat energy. Only a small amount of the PV electricity generated was used by the flat itself, as there were only a few days in which the heating requirements and supply of solar radiation were correlated. This meant that power had to be taken from the grid.

5.2 Flexibility potential of heating grids with heat pumps

Traditionally, district heating systems are operated at high temperature levels. A shift to lower temperatures offers several benefits, such as energy efficiency, sustainability, and the integration of renewable energy and waste heat sources. Often, low-temperature district heating (LTDH) networks contain heat pumps to accommodate the decreased temperature levels. At the FZJ, within the scope of the LLEC, an LTDH network providing the waste heat of a supercomputer to nearby buildings at a temperature of approximately 40°C, is about to be commissioned. The heating grid is formed by disconnecting an existing part of the conventional heating network (originally supplied by a nearby lignite power plant, and since 2023 by a CHP plant on-site) and extending the resulting independent heating network with additional pipes to resolve bottlenecks resulting from the higher mass flows. As the existing building stock has comparably high temperature demands, heat pumps with associated thermal storage capacities were installed in each building and connected to increase the temperature level to the required temperature one of the individual building.

One of the primary research goals is the seamless integration and operation of heat pumps with renewable energy sources as well as waste heat. All buildings connected to the LTDH are also equipped with sensors and heating valve actuators on a room-by-room level. As a result, this setup allows the full real-world flexibility potential to be studied, while making use of the inertia of the network itself, the thermal storage, and the secondary side of the heat pump as well as the inertia of the building, all while incorporating the level of operational freedom provided by the comfort ranges of the occupants. The design of (low-temperature) heating networks is most often formulated as a MILP, in which temperatures and mass flow rates are neglected or simplified. *Hering et al.*[65] described a Mixed Integer Quadratically Constrained Program (MIQCP) with temperature constraints. As a case study, the integration of low-temperature waste heat in a district heating network is optimized. In this case study, the positioning of heat pumps at the waste heat supply or consumer side is optimized. *Hering et al.*[66] employ quadratic correlations to model temperature characteristics for the operation of the district heating network. A MIQCP program is presented that optimizes the operation of heat pumps combined with thermal energy storage facilities and the operating temperatures of a pipe network. In *Liu et al.*[67], the controller was extended by adding constraints for the exchange with the electricity grid. The developed setup was then tested with the help of a Hardware-in-the-Loop (HIL) co-simulation framework to evaluate multi-modal energy systems.

The efficiency of heat pumps depends primarily on the temperature difference between the heat source (primary side) and the temperature required by the building heating system (secondary side). Simply replacing the existing heat source in buildings, mostly fossil-fired boilers, with a heat pump, will result in inefficient heat pump operation and comparatively high electricity demand. Occasionally, changes are made to a building after completion of construction work. These changes might not be captured in the heating curve, which describes the supply temperature on the secondary side as a function of the ambient temperature. By evaluating the actual requirements on the secondary side, it may be possible to reduce the heating curve, which would allow for more efficient heat pump operation. Bottlenecks in the heating system, such as limitations in specific components like radiators, can impede a lowering of the heating curve. By addressing these, the system's performance can be enhanced. However, most estimations of the temperature reduction potential in existing buildings are based on measurement data at the room level or detailed information about the building's physics. In order to reveal the temperature reduction potential for a large number of buildings and thus strive for wide applicability, a novel method was developed at the FZJ that focuses on estimations for feasible supply temperature reductions in existing buildings with limited input data.[68] By evaluating historic heat demand data at the building level, outdoor temperatures and basic information about installed radiators, the minimal actual necessary supply temperature is calculated for each heater in the building using the logarithmic mean temperature difference (LMTD) approach. The overall required flow temperature for the entire building is determined by the maximum required flow temperatures of all rooms at different outside temperatures, resulting in an updated heating curve. This method was applied to multiple existing office buildings at the FZJ, demonstrating its fast applicability. In one building, the heating curve deduced by the novel method was implemented in the building automation. During a first test spanning three days, it could be shown, that it was possible to supply the required heat demand by using the lowered heating curve.

5.3 Occupant-oriented demand response in the building sector

Research at the KIT and FZJ conducted on "Occupant-oriented demand response in the building sector" has focused on relieving stress from the electricity grid while satisfying the occupants' thermal requirements. The DR is a key solution for future electricity grids, where energy use shifts over time. This supports the balance of energy use and volatile electricity production from renewable energy sources, e.g., wind and solar. However, as occupants are responsible for energy demand, their requirements must be carefully considered when shifting electricity.[69, 70]

Buildings are characterized by a significant potential for shifting energy use thanks to their slow thermal dynamics. This potential can be exploited by heating buildings electrically, e.g., from heat pumps, and optimally scheduling this electricity consumption. This scheduling must respect the requirements of the occupant and the electricity grid.

At the KIT, a novel framework, based on MPC, was developed, that considers the electricity grid in terms of a dynamic electricity price and the occupants' thermal requirements by permitted temperature ranges that are time-variable and room-individual. The results indicate the potential to reduce energy costs by approximately 40% compared to conventional control strategies.[71]

The framework calculates an optimal schedule by considering a weather forecast, an electricity tariff, a thermal building model, and an occupancy profile. Neither the weather forecast nor the model are error-free. On the contrary, forecasts and models are subject to uncertainties that lead to deviations from the optimal schedule. We address the uncertainties by means of advanced control strategies, namely stochastic (SMPC) and robust MPC (RMPC), and compare their results against conventional deterministic MPC (DMPC). The results show that forecast uncertainties lead to violations of occupants' thermal requirements with DMPC, whereas SMPC and RMPC fulfill these.[72]

At the FZJ, the development and testing of JModelica[73]- and Python-based scheduling and control frameworks for rooms and buildings under near to real-world conditions is one major research topic. For interactions with users, a web-based dashboard suite was implemented as a monitoring and control interface.[74] Within the scope of the Living Lab Energy Campus (LLEC) initiative, a testbed for the evaluation of novel monitoring and control methods at both the room and building levels has been established.[75, 76] In addition to the retrofitting of hardware in buildings, an information and communication technology (ICT) platform was designed and implemented to form the basis for the execution of the monitoring and control frameworks, as well as the dashboard suite.[77] The different contributions are described in greater detail in the following section.

Inert heating systems such as Thermally Activated Building Systems (TABS) or underfloor heating systems must be activated well in advance in order to cover heating demands. Model-based scheduling and control approaches are well-suited to the control of such thermal systems, as they are able to incorporate information about building dynamics, as well as forecasts with respect to, e.g., weather (ambient temperature, solar irradiance) and occupancy. *Althaus et al.*[78] showed the design and implementation of a cloud-based, configurable room heating control algorithm and investigated the effects on energy demand and occupant comfort in a field test at the FZJ. In *Johnen*[79], the parametrized room models were studied in detail. In parallel, an MPC framework based on Modelica and JModelica was implemented, which allows for both the hierarchical and distributed subdivision of control problems so as to be able to handle large-scale building energy systems featuring components with different time dynamics.[80, 81] In *Mork et al.*,[80] a hierarchical MPC approach was implemented to enable the simultaneous control of actuators of both slow and fast dynamics, which outperforms conventional and non-hierarchical control approaches. The hierarchical MPC consists of two layers: one focusing on slower dynamics and disturbances and one on the faster ones. The structure of the hierarchical MPC concept is shown in Figure 19. In *Mork et al.*[81], time-variant thermal comfort ranges were exploited for multi-zone buildings based on a distributed MPC approach, which exhibited a better performance compared to centralized and conventional control approaches.

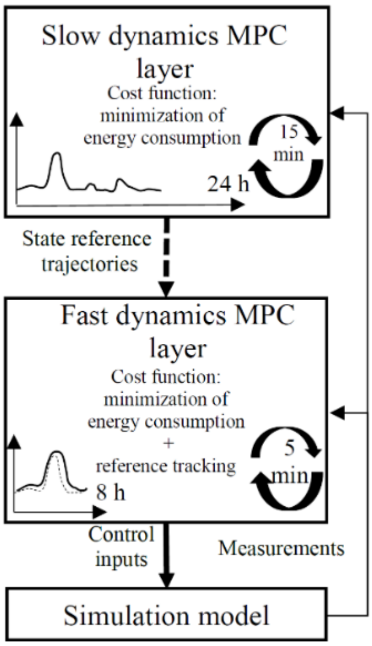

Figure 19. Structure of the hierarchical MPC concept.[80]

In a first real-world application, the developed framework was applied to an office space with a heating system comprising a combination of radiators and underfloor heating, as well as Venetian blinds.[70] Figure 20 displays typical results from this first real-world application of the Modelica-based MPC framework.

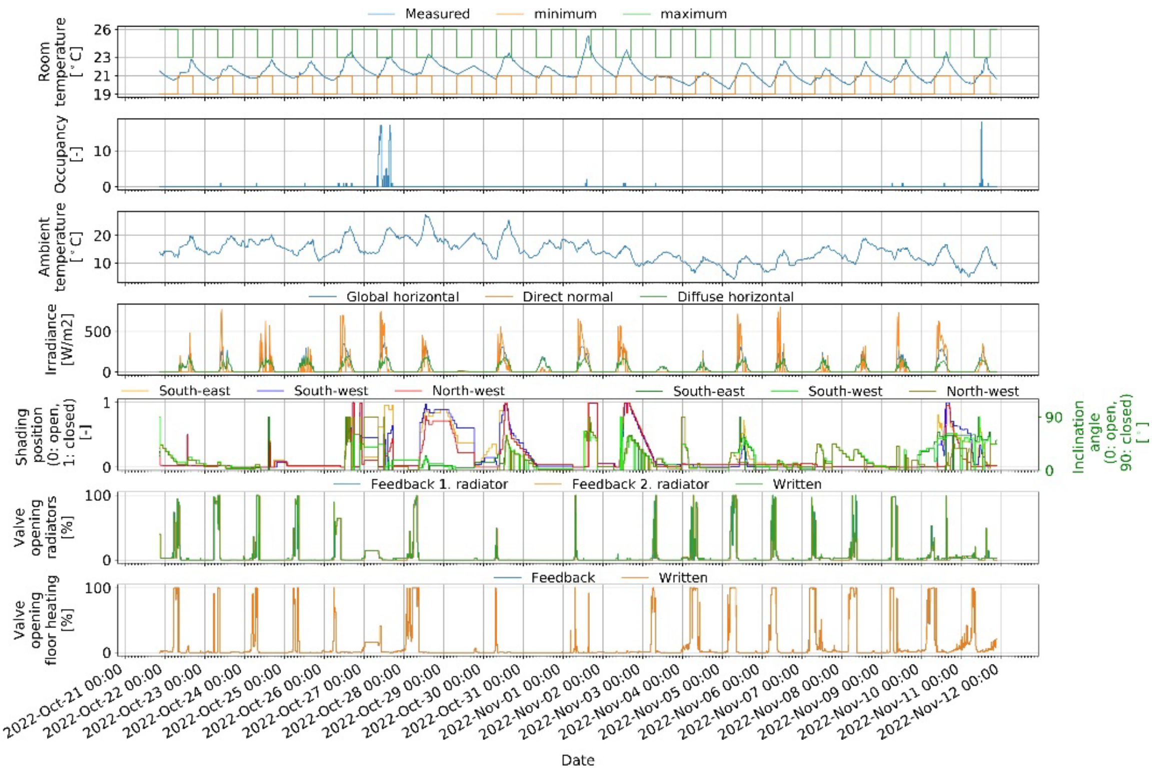

Figure 20. Typical MPC results from the first real-world application of the JModelica-based MPC framework (from October 11 to November 7, 2022).[70]

The results demonstrate that the heating control is well able to keep the room temperature within the given temperature bounds at most times. In addition to this, the controller operates the room temperature in an energy-efficient manner near the lower temperature bounds, exploits the higher energy efficiency of the floor heating, and heats the different actuators according to their dynamics to provide thermal comfort at the beginning of occupancy periods.

The developed framework integrates software modules for forecasting weather quantities and occupancy. The activation of the thermal mass of a building with high potential inertia allows for its use as passive storage to shift the times of energy supply and demand. The passive storage capacities could also be transferred to the control of air quality (e.g., in the form of CO_2 concentration) by keeping air quality below the upper bounds during occupancy periods.

To exploit the full flexibility potential of buildings by means of the thermal inertia without negatively affecting user satisfaction, the consideration of the building occupants and their individual comfort preferences is a key factor. Within the scope of the LLEC initiative at the FZJ, a dashboard suite has been developed to increase awareness of employees for energy-efficient behavior at the office level by providing insights with respect to energy demand and indoor air quality-related measurements and derived values.[74] The web-based application JuControl allows occupants to control, e.g., the temperature in their office via the dashboard manually (by manually providing a temperature set-point) or automatically (by specifying their personal temperature preference range and time schedules of expected presence). Figure 21displays screenshots of JuControl, showing the measurement data and control interface, as well as a “presence calendar,” which displays the anticipated presence in the office of an average user.

If the office is unoccupied for a longer period of time, the permissible temperature range is further extended beyond the one defined by the occupant(s). By incorporating this additional data in the (model-based) room controllers, the flexibility potential can be further increased without harming user comfort. In case the heat is provided by an electrified heating system (e.g., a heat pump), the increased flexibility on the thermal side offers additional flexibility potential to the electricity grid. The comfort ranges for the room air temperature can be regarded as passive thermal storages that can be charged or discharged, depending on the current states of the room temperature, electricity grid, energy prices, coefficient of performance (COP) of a heat pump, and occupancy forecasts, for example. In addition to the flexibility potential, with the help of the equipped buildings in the LLEC, the extent to which gamification can increase occupant energy awareness and thus lower energy demands and load on the electricity grid is analyzed.

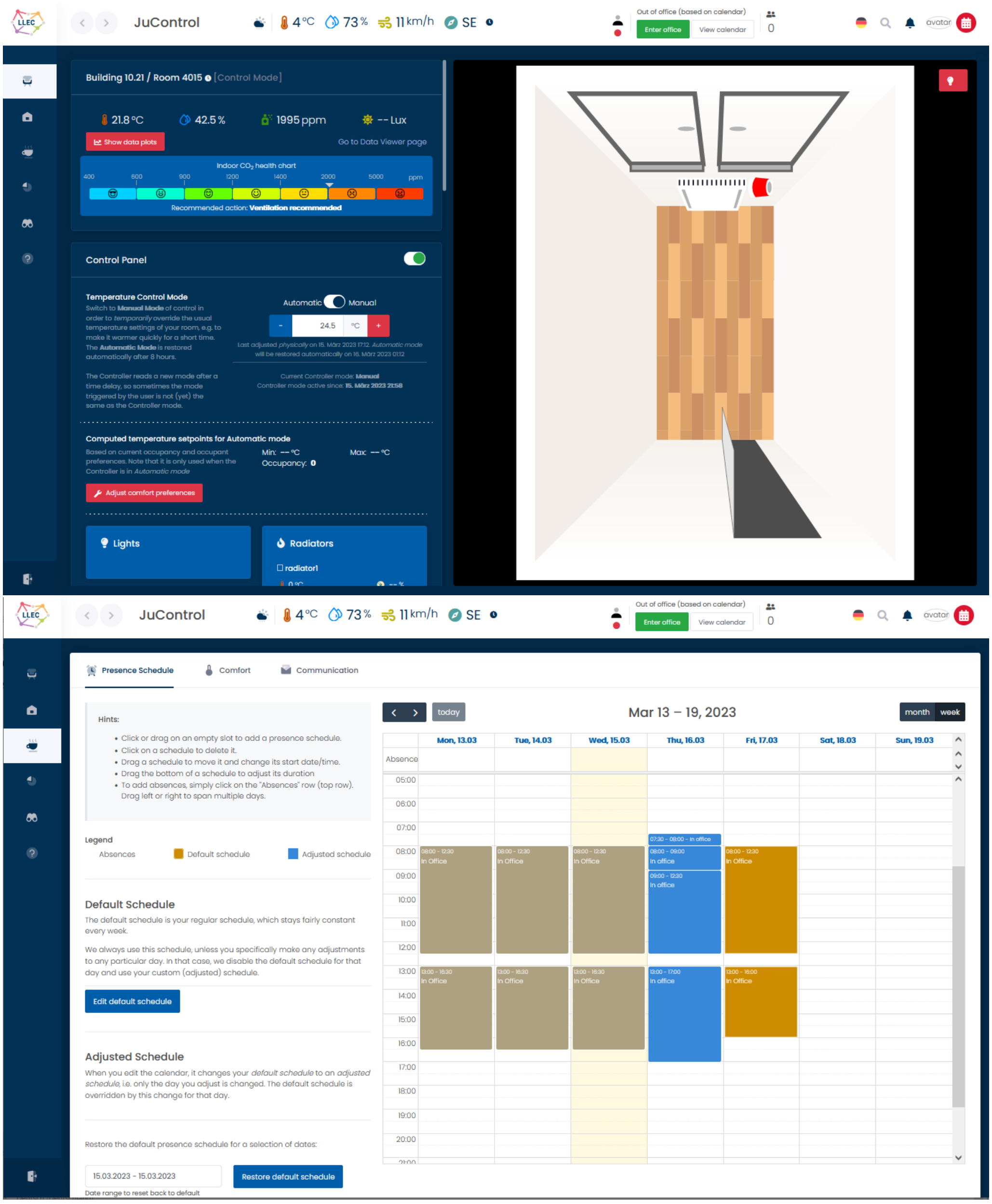

Figure 21. Screenshot showing the main page in JuControl, displaying measurement data and the control interface for a typical office (top); screenshot of a "presence calendar," showing the anticipated presence in the office of a typical user (bottom).[74]

Accurate information regarding the current room state, e.g., temperatures, CO_2 concentration, and illuminance, is crucial for calculating the optimal setpoints for, e.g., heating and shading systems in order to provide thermal and visual comfort and maintain good air quality. Thus, sensors and actuators, including the corresponding ICT infrastructure, are an essential prerequisite for the practical implementation, demonstration, and evaluation of advanced automation and control methods. As part of the LLEC initiative at the FZJ, to date, 15 existing buildings have been equipped with a comprehensive and scalable (research) infrastructure for building monitoring and control based on different non-proprietary protocols.[75]Thus far, over 500 offices with more than 750 unique users have been equipped. This large sample size contributes to the statistical significance of the experiments carried out. The experimental setup will be extended in the near-term future by a new building currently under construction, which is planned to be climate-neutral during operation by design, and the consequent application of model-based planning and scheduling methods on multiple levels. This new building will be connected to the low-temperature district heating (LTDH) network currently being commissioned and features a combination of convectors and TABS with a high thermal inertia. Once put into operation, the demand-side flexibility of this building will be assessed in detail.

The setup established in the LLEC enables the demonstration and evaluation of both (cloud-based) room-level monitoring and control, as well as building-level automation. In order to guarantee the security of supply and comfort of rooms, the system is designed in such a way that it is possible at all times to switch to a default (non-scientific) operating mode. Multiple mechanisms such as “kill switches” are implemented, which can be activated manually or automatically in case of malfunction. A malfunction is defined, e.g., by the violation of a threshold or by a suspension of the heartbeat signal of a vital system component or micro-service.

One of the defining characteristics of the building sector is the uniqueness of each structure. Unlike mass-produced products, buildings are typically designed and constructed to meet individual requirements, taking into account specific factors such as location, purpose, budget, and architectural considerations. As the construction rate in Germany is less than one percent per year, the monitoring and control methods developed must be applicable to existing buildings in order to achieve a significant near-term impact. The frequent lack of proper and up-to-date documentation for existing buildings can pose significant challenges for the implementation of, e.g., model-based scheduling approaches, which heavily rely on an adequate model of a building. Even if documentation is available, depending on the year of construction, it only exists on paper or does not have the correct data format. Furthermore, planning companies generally do not have the knowledge to develop the required models. Thus, one of the key challenges for the broad adoption of the developed monitoring and control approaches is the easy, fast, and affordable generation of building models.

A promising way to solve this problem is the automated generation of models from statistical or cadastral data. The KIT is therefore researching methods for enriching existing data to create building models that allow energy simulation and optimization.[82, 83]

At the FZJ, model generation is addressed by multiple developments: A user-friendly and universal mini-language, ALICE, has been developed with the aim of capturing the main characteristics of rooms (thermal zones) by describing their main dimensions and position, as well as the dimensions and main characteristics of heaters, walls, doors, and windows with minimal effort. Especially with repetitive patterns, as often feature in office buildings, it is possible to describe entire large-scale buildings with little effort. Based on the description of a room, a graphical representation in a pseudo-3D top-down view can be generated to form the basis for measurement data visualization to users in the web application, JuControl. At the FZJ, for generating models (digital twins) of buildings, the Modelica simulation model library AixLib [84] is used as the basis for creating physics-based models as a starting point. *In Mork et al.*[85], a newly-developed toolchain is described, which, based on ALICE, generates white-box simulation and controller models for both thermal zones and entire buildings in the modeling language Modelica, utilizing components of the open-source AixLib model library. In parallel, gray-box approaches are pursued. In an iterative calibration method, a parameter estimation approach adjusts selected model parameters based on measurement data gained from building operation.[70] All rooms that have been equipped with sensors and actuators within the scope of the LLEC have been captured in the ALICE language. In the next step, with the help of the white-box simulation models, the increase in the flexibility potential of office buildings by incorporating data regarding future room occupancy patterns in control systems for buildings with different building envelopes will be assessed in detail.

The research outcomes provide valuable insights for the implementation of demand response strategies in the building sector, offering a robust framework for the design and control of energy-efficient buildings. Overall, it could have a profound impact on advancing automation technologies and enhancing the sustainability of urban environments.

5.4 Decentralized heat and power generation for buildings using hydrogen

This section focuses on the question of which technological advancements will be needed in order for hydrogen-powered (mobile) fuel cell systems to be used as a decentralized option for generating electricity from hydrogen and how by-product heat can be used efficiently during this process.

Technological solutions for integrating the two energy sectors of power and heat with the transportation sector are being evaluated as part of the project, EVer ("Energie und Verkehr" = "Energy and Transport").[86] The DLR is developing technologies at the interface between vehicles and the electricity grid. In the case of fuel cell–electric vehicles, the generated by-product heat also enables an interface with the heat sector.

Researchers are increasingly focusing on technological enhancements to decentralized hydrogen-powered fuel-cell systems (particularly mobile fuel cell–electric vehicles and stationary CHP plants) in light of the options that they offer for generating electricity from hydrogen, their efficient use of waste heat, and the possibility of incorporating air conditioning and central heating into the hydrogen-to-electricity process. Technological solutions for integrating the power, heat, and transport sectors are being investigated in the EVer project. As part of the project, therefore, the DLR is paving the way for two interfaces required for cross-sectoral integration: feeding electricity from the vehicle back into the grid and the utilization of waste heat inside the building.

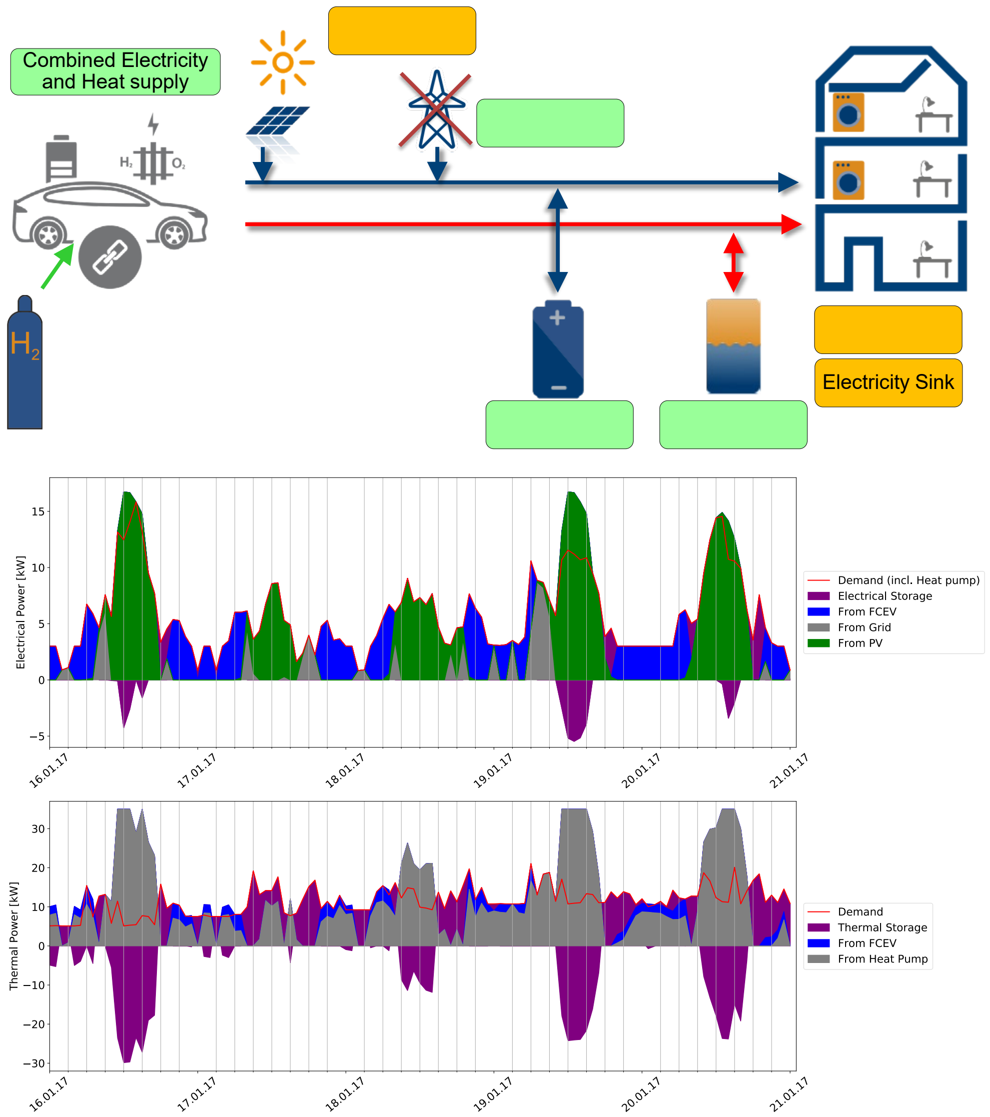

Figure 22. Graphic representation of the "oemof" optimization model used, which connects a building and vehicle via an energy interface (top). Calculation in oemof for feeding electrical energy from a parked fuel cell car back into a single-family home.[87]

As well as increasing the overall energy efficiency of the energy source/fuel used, i.e., hydrogen, decentralized integration of the transport sector will also enable energy for the electricity sector to be supplied much more flexibly. A network of many vehicles in a future "virtual power plant" would therefore be able to replace the existing fleet of backup power plants while meeting transportation and heating demands at the same time. Simulations using a fuel cell–electric vehicle to cover the electricity and heating requirements of a single-family house were run using the oemof open energy modeling framework. As an example, the results for electricity fed back into the building are shown in Figure 22. In the simulated arrangement, up to 100 percent of the electricity required for single-family houses could be covered by using no more than 3 kg of hydrogen from the vehicle. The demand for heat and hot water cannot be fully met in the winter months, as the need for heating significantly exceeds that for electricity. Current simulation models are looking to use several fuel cell–electric vehicles for apartment buildings during the dark doldrums.[88, 89]

Against this background, a test facility has been developed that is capable of extracting the electrical energy generated by the vehicle and feeding it into the electricity grid while also processing the waste heat generated in a thermal building emulator (Figure 23).

Figure 23. Test facility for the integration of fuel cell–electric vehicles into households. Quelle: DLR

The use of electricity sources/sinks allows representative electrical load profiles in buildings to be reproduced flexibly. Power outputs of up to 11 kW can be adsorbed by the sinks. The test facility is also equipped with interfaces for CCS, ChaDEMo, and type-2 AC connectors. This will allow bidirectional electrical power flows to be represented and mapped in both AC and DC in the future based on current charging standards.

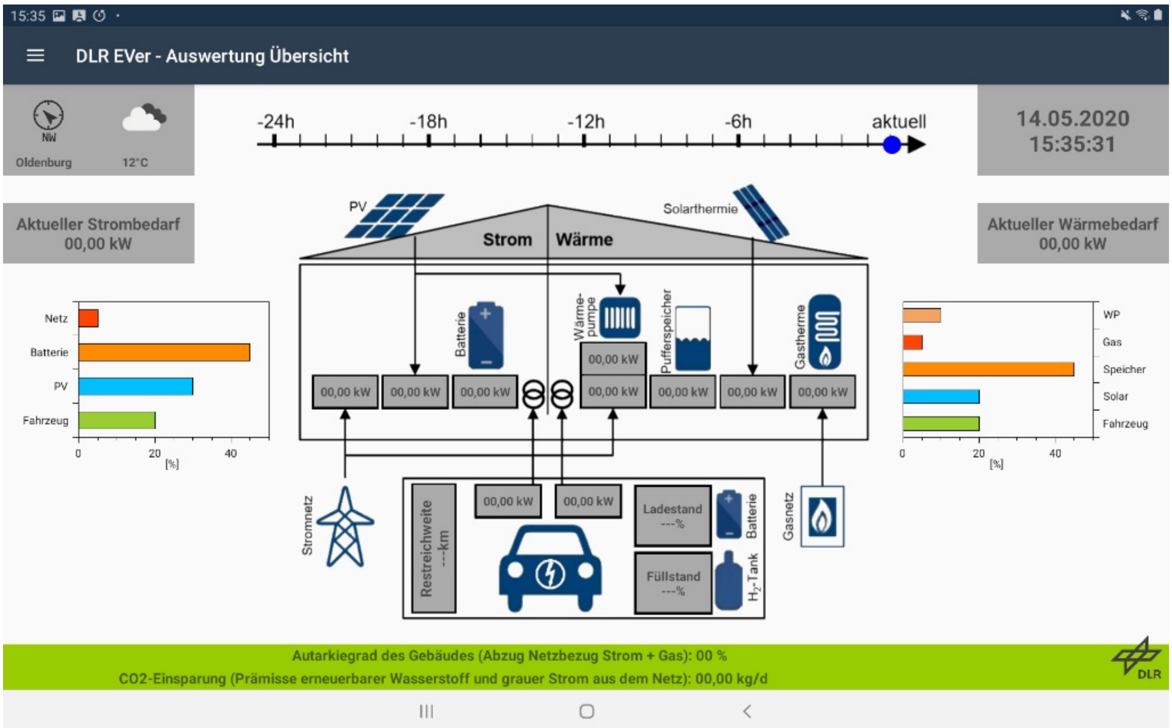

Figure 24. An app allows the power flows inside the complex "vehicle/building" system to be visually represented in real-time.

A Bluetooth-based, encrypted real-time communication environment was implemented for transferring information on the current operating states of the vehicle and test facility in order to regulate and illustrate this complex and integrated “vehicle/building” system. Using an app (Figure 24), power flows can be displayed in real time for the user and – in an enhanced version – for developers as well.

The data transmitted from the vehicle are read off through a special measurement sensor system provided by the DLR as well as via the standard CAN bus in the vehicle. This is done so that validated measurement data can be generated and help to enable simulation models to work more realistically and in greater detail. Two key questions here are how much heat can actually be fed into the building and what conclusions can thus be drawn for future implementation efforts.

Decentralized, stationary CHP plants in the low-performance class with low electrical output incur higher specific investment costs and thus take longer to pay for themselves. If such plants are to be operated economically, their use over the runtime must be as long, maintenance-free, and low-degradation as possible. Aspects of the durability and electrical and combined (heat and power generation) conversion efficiency of CHP systems in buildings were therefore investigated as part of the national joint project LifetimeINH5000 and the European project D2Service.[90] This revealed that system components and their integration and operating mode have a significant impact on durability and efficiency. This durability and efficiency can be improved by reducing degradation and optimizing components and/or operational management concepts (Figure 25).

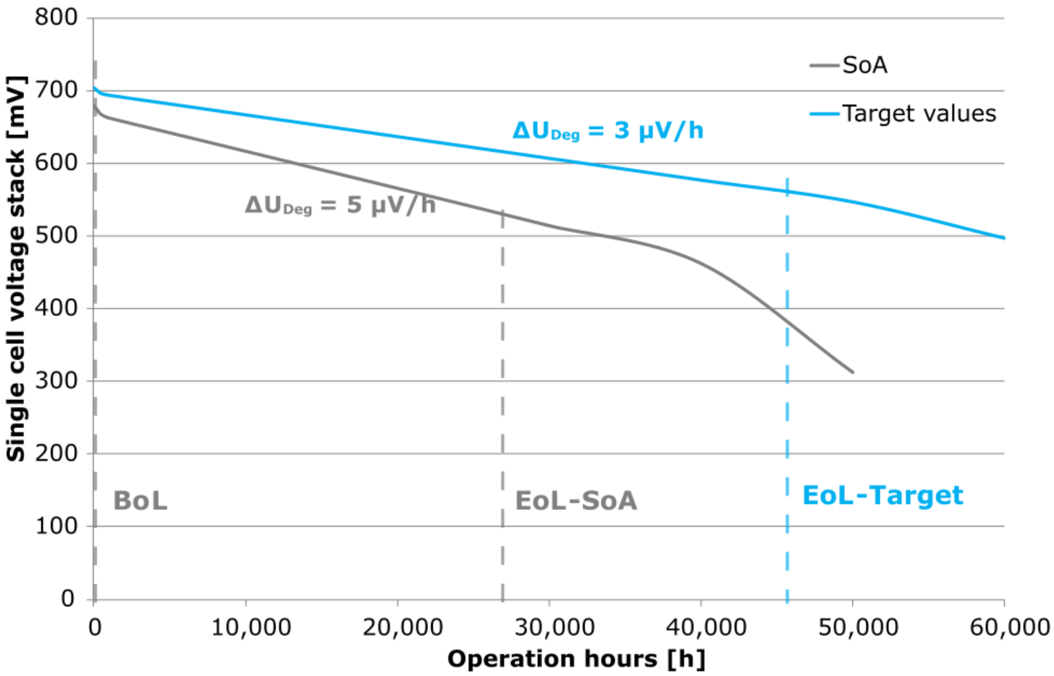

Figure 25. Examples of cell voltage curves from the Lifetime project.

Degradation effects at the stack and reformer are being studied at the DLR by operating a CHP test bench integrated into the building system under realistic conditions in the test facilities constructed specifically for this purpose. Models are being developed and used at the cell and, in particular, the system level in order to design a solution in a targeted way. To validate the durability and efficiency of CHP plants, test procedures were devised that enable the subsystems to be operated under realistic conditions. The solutions developed were transferred to the system level and demonstrated in an endurance test of about 5,000 hrs. Figure 25 shows the cell voltage curves inside the fuel cell stack for a PEMFC CHP plant at different rates of degradation (gray curve: state of the art; blue curve: target). The stack voltage shows a linear decline over operation time until around 38,000 operating hours, after which the degradation rate further increases (gray curve). However, in real-life operation, this point is never reached ("end of life" criterion).

The project is geared towards reducing the rate of degradation and increasing durability accordingly by optimizing the stack and overall system in various ways (blue curve). Figure 25 shows the overall conversion efficiency of a (solid oxide fuel cell) SOFC CHP system depending on the usable temperature level inside the buffer storage system. This is largely determined by the thermal conversion efficiency and reduces as the temperature rises, as is to be expected.[90]

The aspects of the durability and efficiency of integrated CHP plants are currently still being systematically investigated in the projects with respect to natural gas-powered systems. The first investigations into the direct use of hydrogen have already improved degradation and efficiency. However, the results obtained and methods devised can still be transferred very effectively to operating methods and intelligent operating regimes using hydrogen instead of natural gas.

Table 1. System used to categorize typical days.[91]

Season	**Daily temperature Daily average**	**Working days**		**Sundays**	
		Bright	Cloudy	Bright	cloudy
Winter W	T_{mittel}<5°C	WWH	WWB	WSH	WSB
Summer	T_{mittel}>15°	SWX		SSX	
Transition	5°C≤ T_{mittel}≤15°C	ÜWH	ÜWB	ÜSH	ÜSB

Coverage	**Criteria**
Bright H	Coverage <5/8
Cloudy	Coverage ≥5/8

The integration of a fuel cell system into a building that generates heat and electricity using hydrogen requires detailed knowledge of the building's load profiles for the purposes of system integration and interface design – regardless of whether a stationary or mobile fuel cell system is involved. New reference load profiles for single-family houses with nuanced load profiles in terms of their electrical energy demand for household use, room ventilation, and general needs were produced as part of the VDI–RefPro and in particular the NOVAREF project. All of these single-family houses are low-energy homes. These benchmark load profiles are an essential prerequisite for producing reliable load profiles for models of buildings and residential districts, as they enable interfaces with decentralized heat generation and hydrogen-to-electricity plants to be reliably designed.

The benchmark load profiles were produced based on comprehensive monitoring measurements taken from real-life single-family houses over the course of a multi-year project, which in some cases is still ongoing. The data are anonymized for further use. The individual daily datasets are allocated to so-called categories of type days (Table 1) based on calendar and climate criteria that have been specifically chosen. This is done using a method in guideline VDI 4655[91] that describes such an approach and provides ready-made benchmark load profiles. The daily curves were normalized to enable a representative daily load profile to be selected for each benchmark day and each building from the many daily datasets available (Figure 26).

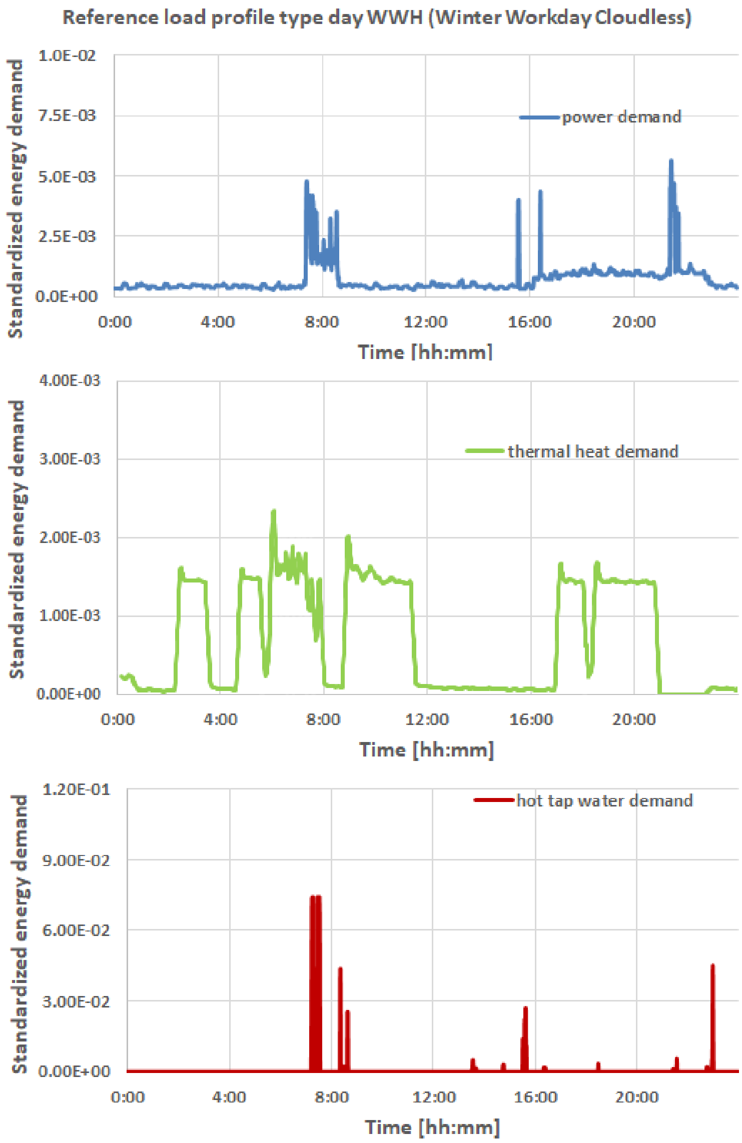

Figure 26. Representation of a daily load profile for the benchmark day entitled, "Working day, winter, no cloud cover" in accordance with VDI 4655.[91]

Another study in terms of the combination of CHP Systems and heat pumps in a low-voltage distribution grid was conducted by *Ahmed et al.* as part of the SDK2050 project. The study introduced a set-up for using power hardware-in-the-loop for the validation, inclusion, and characterization of hydrogen-based components (e.g., CHP systems). The study pointed out that a mix of CHP units and heat pumps in the neighborhood can meet the heating demands of its households on the one hand and, on the other, help to stabilize the low-voltage distribution grid.[92]

5.5 Design and layout of innovative energy systems on the district level

Developing sustainable energy supply systems for residential districts and properties requires numerous different aspects to be considered. For instance, the increasing integration of the electricity, heat, and transport sectors must be considered just as much as the seasonal dynamics of energy provision and local conditions, such as existing grid infrastructures, transport links, and the condition of existing buildings. To tackle these challenges, the DLR determined the basic concepts of planning tools for integrated energy systems on various spatial levels and time-scales. On the one hand, a model was developed that allows realistic energy models of urban structures to be created based on publicly-available data. On the other, a modeling environment for "installation-specific energy system design" was created that allows the design and layout of installations to be optimized with respect to several KPIs.

Developed at the DLR, FlexiGIS ("Flexibilization in Geographic Information Systems") is an open-source, open-data tool for modeling and optimizing urban energy systems[2]. Such open-energy models lend support to the decision-making process at the policy level by providing relevant insights into the planning of sustainable districts and cities. However, open energy models and freely-available, reliable data sets are rarely provided with the required level of detail.[93] Therefore, FlexiGIS contributes to the open modeling of urban energy infrastructures.

The FlexiGIS tool is designed to be modular and transferable and can therefore be used by a broad target group of users. The spatial and temporal distribution of local electricity consumption, as well as its local power generation, are simulated in FlexiGIS. The tool makes use of GIS techniques and allows the integration of different datasets. These can be further linked to additional layers of data such as land use or any desired installation locations.

A bottom-up approach is adopted to calculate electricity demand and generation at high spatial resolutions based on building and road prototypes (see Figure 27 for an example of the high level of detail that can be obtained for building classification). The geo-referenced data of building and road prototypes was extracted from the OpenStreetMap database.[3] The developed model has been successfully validated using measurement data provided by EWE NETZ, the local distribution grid operator.[94] In order to investigate various scenarios for deploying flexibilization options such as power storage systems in urban environments, an optimization was conducted using FlexiGIS via a soft coupling between FlexiGIS and the urbs[4] optimization model.[95-97]

[2] https://github.com/FlexiGIS/FlexiGIS
[3] https://www.openstreetmap.org/
[4] urbs: A linear optimisation model for distributed energy systems — urbs 1.0.0 documentation; GitHub - tum-ens/urbs: A linear optimisation model for distributed energy systems

The open-source, open-data approach of FlexiGIS proves that (urban) energy systems with freely accessible data records and tools can be realistically represented using freely-accessible datasets and tools.[97, 98] In addition, the open-source approach also helps to increase the modeling transparency and acceptance of the results amongst various stakeholders.

The use cases investigated using FlexiGIS have shown that higher degrees of self-sufficiency can be achieved in urban settings by increasing the percentage of integrated renewable energy sources in the power supply system.[94-97] As the share of decentralized renewable electricity generation in cities increases, the storage of electricity is of the utmost importance. The optimization results from the case studies indicate that a high percentage of renewables (up to 60% of installed power) by 2030 could cut overall system costs in half compared to today's energy system costs. Nevertheless, an "off-grid" scenario or a fully self-sufficient urban energy systems is neither cost-effective nor technically-feasible.[94, 96, 97]

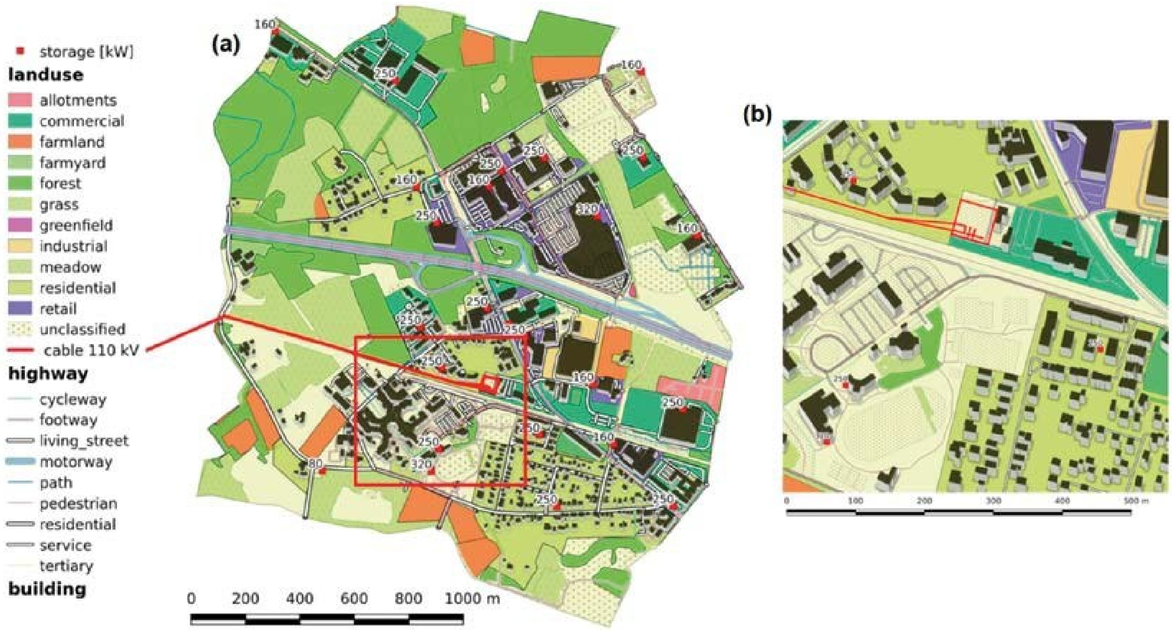

Figure 27. Cartographic representation of the urban energy infrastructure and potential locations for decentralized battery storage systems in a scenario for 2030 for the Wechloy district of Oldenburg (a). The enlarged area (b) shows the energy infrastructure and the distribution structures for battery storage systems.[96]

In addition to covering the electricity sector, the first results of integrating the heat sector into the FlexiGIS tool were achieved. The potential assessment for integrating geothermal heat pump technologies in an urban setting was also conducted.[99] In this first work, we compare ground-source and aerothermal heat pump usage in various integration scenarios. An open dataset providing the energy potential and locations for geothermal systems was generated for the city of Oldenburg. FlexiGIS was used to estimate thermal energy consumption based on the city's building infrastructure. We evaluated the data utilized by various geothermal systems and used performance coefficients of aerothermal and geothermal heat pumps to project power and energy consumption across three energy scenarios. The findings indicate that borehole heat exchangers (BHEs) and ground-source heat pumps (GSHPs) represent the optimal choices for deploying shallow geothermal systems within urban areas. Their efficiency, compact spatial demands, and reduced impact on electricity grids make them a superior option compared to air-source heat pumps. Shallow geothermal energy (SGE) can present a cost-effective and eco-friendly substitute for natural gas when it comes to heating spaces and providing hot water. Nevertheless, the adoption of GSHPs comes with certain challenges, including technical and non-technical obstacles, environmental concerns, and limitations in historic structures.

The “Model template for residential energy supply systems” (MTRESS), developed at the DLR, is a modeling tool for the easy creation of energy system models of sector-integrated systems (not exclusively residential) that integrates electricity, heat, hydrogen, and natural gas as energy carriers, including the quality of the energy, e.g., its temperature profile.[100] It then optimizes the operation of the components in the system. MTRESS is based on the open-source software, oemof.solph[101], which was developed by an inter-institutional community, with a majority of the latest major contributions originating from the DLR.

MTRESS facilitates conducting studies scanning a large solution space, i.e., various different configuration of energy systems, for (Pareto-) optimal solutions considering multiple conflicting performance indicators.[102] In *Hancock et al.*[103], Pareto-optimal (in terms of costs and emissions) renovation strategies for residential buildings from various (thermal insulation and technical building equipment) of different construction years, based on data from the TABULA database, were identified.

By using the performance indicators of energy systems for varying input data, MTRESS can be used to identify universal energy supply systems. In *Schönfeldt et al.*[104], this approach was used to identify optimal energy supply systems that can be implemented for standardized buildings in different climate regions. With Version 3, MTRESS was extended by the concept of locations (for concept description, see *Lesnyak et al.*[105]). This enables the simulation of multiple interconnected nodes with individual energy supply systems.

For operation optimization, MTRESS can be used on the basis of short-term forecasts as input data.[106] Using a rolling horizon approach with a suitably short time period, the MTRESS was used in an MPC-style algorithm for an optimal control strategy for a district energy management system.[107]

At the FZJ, the overall campus supply of cooling, heating, and power was evaluated in a study that analyzed the integration of waste heat from a new high-performance computer[108] In this work, the energy system model for the campus was modeled using the COMANDO framework[60] and optimized in a simultaneous design and operational optimization. Several energy supply systems were considered, such as CHP plants, heat-only boilers, adsorption, and compression chillers and heat pumps for increasing the waste heat temperature. A bi-objective optimization was conducted to ensure that the heating, cooling, and power demands were met while balancing the global warming impact and total annualized costs subject to different gas-to-electricity price ratios.

6. Transport

Furthermore, decentralized flexibilities can be created by integrating electrified vehicles into the electricity system. The controlled charging of battery–electric vehicles could relieve the distribution electricity grids or provide load flexibilities to the electricity markets. In the future, it would also be conceivable to feed electricity back into the grid during peak load periods by allowing bidirectional charging, i.e., vehicle-to-grid. When the share of electric vehicles increases, these flexibilities are highly welcome in the electricity system.[109-111] Hence, the flexibilities from electric vehicles may play a major role in the electricity system – still depending on user acceptance.[112]

Another dimension of flexibility could come from the decentralized connection of fuel cell vehicles to the electricity system. This also has the effect of increasing the overall system efficiency, as it is also possible to use the waste heat, for example, to supply buildings. Here, the power class (e.g., passenger car, truck, or rail vehicles) essentially determines the level and scope of the services that can be provided, especially if these are coupled with a hydrogen supply and a power (electrical and heat) reconversion infrastructure. The DLR is researching basic approaches to the connection and design of interfaces for this purpose in a joint effort with different Helmholtz programs.

In the transportation sector, research has been conducted for several decades on the use of hydrogen – both in connection with fuel cells and for direct combustion. Apart from the higher efficiency compared to hydrogen combustion engines, its use in fuel cells has the advantage that apart from water, no other emissions are produced. There is a global standard for the refueling and storage of hydrogen as a compressed gas, which generally provides 350-bar systems for buses, heavy-duty, and rail vehicles. 700-bar systems are primarily used in passenger cars, as well as applications in which a higher energy density must be achieved at the storage system level due to limited installation space. Compared to a battery, the combination of fuel cells and hydrogen storage has a more favorable gravimetric and volumetric energy density. For this reason, more research is currently being conducted in the areas of heavy-duty trucks, maritime systems, and short-haul flights. By processing hydrogen into synthetic fuels – also called "electricity-based" or "e-fuels" – even high-performance applications can be made climate-neutral through the use of renewable energy sources.

6.1 Individual transport

Hence, personal or individual road transport with battery– or fuel cell–electric vehicles offers great potential for electrical flexibility in the grid. It is known that vehicles in passenger transport are only used for driving for a small portion of the time, which is why the application here is obvious (<5% of the time, they are used for driving; they always make up about half of the available vehicles parked)[113]– again, these values might be significantly lower due to fewer plug-in times. In purely mathematical terms, 10 million parked and connected vehicles feeding into the grid at the same time are sufficient to provide 100 GW of electrical power for the grid (assuming a three-phase, 16 A connection of ~11 kW), which is much more than the average current peak demand of a German household – and additionally, the correlation in time (simultaneousness) for charging is much higher.[114] Due to the long idling times the energy demand – on average about 80% of an average household – can also be distributed over a longer time horizon at much lower loads. When these vehicles are v2g-ready and are also equipped with already-available v2g-ready charging stations, these load flexibilities are tremendous, i.e., about three times higher than their actual daily demand (e.g., a reserved battery capacity of about 20 kWh per household).

As already described in the above chapter on infrastructure and metering, FCEVs are also suited to providing a backup power plant solution in the case of low renewable generation, as the hydrogen fuel is produced seasonally and can be stored in caverns in quantities relevant to the overall energy supply and used accordingly when required.[89] With BEVs, on the other hand, only the energy stored in the vehicle is available and therefore cannot be recharged during longer periods of low renewable generation. For reasons of keeping energy for the mobility demand and for a low wear of the battery, it is likely that only a window of between 40% and 70% (state of charge: SoC) will be used for the bidirectional flexibility. This results in a 60 kWh battery, which is in the range of mid-sized electric vehicle with 300–400 km ranges, in 20 kWh of useable energy, respectively, for a duration of 30 minutes at a power of 10 kW feed-in. Considering local use, on a cold winter day this would be roughly enough energy to supply an average, thermally-insulated, single-family houses with a heat pump for up to two days. Comparing the flexibility of 10 million bidirectional vehicles (~200 GWh) with the current pumped storage power plants (~40 GWh), it becomes clear that this is already a significant value of flexibility if used for grid stabilization. This synergetic integration of EV leads to the simplified integration of renewable energy generators, which in turn decreases CO_2 emissions in the electricity system.[111, 115]

One point that is rarely considered currently is the self-consumption of vehicles when the electronic systems for charging and discharging are on. The cars tested so far had a consumption of 250–500 W, which makes it clear that charging below a certain power level is not useful.[116] This is likely also the reason why the minimum charging power is around 1 kW, which means that 50% is lost in the self-consumption. The same is valid for covering the base load of a building, which is often in the range of 30–200 W. Having this in mind, current vehicles are more appropriate for delivering a power level that is at least ten times higher – and using a stationary storage device for equalizing the load. Finding the right topology or optimization for that will form part of future investigations. The topology of how to connect the bidirectional vehicles to grids on a technical level still remains partially unanswered – even though the technology is already available.

Furthermore, it is currently not fully known how the control of these mobile (or quasi-stationary when parked) generators will be communicatively integrated into building or quarter energy management systems, and who will have the authority of control: vehicle, building, or grid. Here, a harmonized, secure, and safe topology must still be developed to connect all devices. From the Internet of Things (IoT), or the Industrial Internet of Things (IIoT), which is more secure, parts of the control and information exchange could be taken as an example. Yet, the combination with the grid and EVSE communication must be combined.

6.2 Maritime applications

Shipping is responsible for around 3% of global CO_2 emissions. Reduction targets are required to achieve the goals set out in the Paris Climate Agreement. This target cannot be achieved if conventional fuels are used today. Hydrogen, amongst other options, is considered one of the most promising candidates for a zero-emissions fuel. Concerns have been raised, however, about its safety of use and storage. "Safety" is defined as the control of recognized hazards to achieve an acceptable level of risk. In addition, the physical characteristics of hydrogen as a transport fuel may pose a hazard.[117]

To deploy renewable fuels in a global economy, infrastructure and land are also important for enabling the international transportation of goods and fuels. Digital Twins (DTs) play an important role in current digitalization trends across industries. As maritime markets are particularly affected by ongoing global trends such as rising supply costs or political pressure for decarbonization, digital solutions could provide important support to ship-building and shipping companies for addressing current and future challenges.[118]

The backbone of ports must also be developed. As has been seen in the last two years, a hydrogen-capable gas infrastructure has been created to connect the port in Wilhelmshaven with an appropriate storage infrastructure for gases in caverns. This connection is relevant to being able to temporarily store the contents of tanker ships in a direct land connection.

6.3 Hydrogen infrastructure for transport

Hydrogen storage and compression at refueling stations currently requires a lot of energy, especially for personal transport, with pressures of up to 700 bar (900 bar at refueling stations). Alternative liquefaction methods are energy-intensive and require about 15–30% of the hydrogen energy content, and also entail constant losses due to thermally-induced boil-off effects.

An energy-efficient and compact solution to hydrogen storage can be realized with metal hydrides, or more precisely metal–hydrogen compounds. Compared to high-pressure hydrogen storage, twice the volumetric capacity can be achieved at much lower pressures. Especially for stationary use, e.g., in urban areas, metal hydride storage systems therefore have a much smaller space requirement. The storage of hydrogen is 100% reversible, but requires designs that are tailored to the respective application with regard to storage and withdrawal capacity and suitable heat management, as heat is generated during storage and required during withdrawal.

Based on metal hydride storage, a digital Smart-Energy-Transform-Box (SET-Box) was modelled to combine electricity and heat, as well as hydrogen generation and usage. Such a system can be used modularly – and therefore is scalable – as well as in a decentralized manner at different locations. Within the SET-Box, hydrogen can be produced by an electrolyzer and, after passing through a membrane drying process, stored compactly and safely in a metal hydride storage tank or fed into the natural gas grid, and also withdrawn as needed. For withdrawal from the gas grid, efficient polymer-based membranes for the coarse separation of natural gas and hydrogen and again metal hydrides for the fine separation are to be tested. In addition to use in fuel cells, hydrogen from the intermediate storage can also be delivered to other systems at higher pressure levels via metal hydride compressors and used, for example, to refuel vehicles (trucks, cars, ships, etc.). The SET-Box thus enables a flexible transformation of energy and can reliably couple electricity, gas, and transport grids in a grid-serving manner. By mapping the overall concept in parallel with digital twins, the fundamental material laws and the desired application profile in the overall system can be linked across different scales.

7. List of abbreviations

AC	Alternating current
ANN	Artificial neural network
BEV	Battery–electric vehicle
BHE	Borehole heat exchanger
CAN	Controller Area Network
CCS	Carbon dioxide capture and storage
ChaDEMO	CHArge de MOve
CHP	Combined heat and power
CO2	Carbon dioxide
CSTR	Continuously stirred tank reactor
DA	Day-ahead
DC	Direct current
DMPC	Deterministic model predictive control
DR	Demand response
DRC	Dynamic ramping constraint
DT	Digital twin
EI-MS	Electron impact mass spectrometry
EMS	Energy Management Systems
EoL	End of life
ESD	Energy Systems Design
EV	Electric vehicle
EVSE	Electric vehicle supply equipment
FCEV	Fuel cell–electric vehicles
FCR	Frequency containment reserve
FMU	Functional mockup unit (standardized software module)
GPM	Generalized process model
GSHP	Ground-source heat pumps
HDS-LEE	Helmholtz School of Data Science in Life, Earth, and Energy
HESS	Hybrid energy storage system
ICT	Information and communication technology
ID	Intraday
IIoT	Industrial Internet of Things
IMR-MS	Ion molecule reaction mass spectrometry
IoT	Internet of Things
KPI	Key performance indicator
LLEC	Living Lab Energy Campus
LTDH	Low-temperature district heating network
LMTD	Logarithmic mean temperature difference
MILP	Mixed-integer linear program
MIMO	Multiple input multiple output
ML	Machine learning
MPC	Model predictive control
MTET	Materials and Technologies for the Energy Transition
MTRESS	Model template for residential energy supply systems
NF	Normalizing flow
NMPC	Nonlinear model predictive control
PCA	Principal component analysis

PEMFC	Polymer electrolyte membrane fuel cell
PRL	Primary control power
PV	Photovoltaic
RL	Reinforcement learning
RMPC	Robust model predictive control
RTN	Resource task network
SBM	Scale-bridging model
SDS	Simultaneous dynamic scheduling
SET-Box	Smart-Energy-Transform-Box
SGE	Shallow geothermal energy
SI	System identification
SISO	Single input single output
SMPC	Stochastic model predictive control
SoC	State of charge
SOFC	Solid oxide fuel cell
TAB	Thermally-activated building systems
TABULA	Database
TOR	Thermal energy to operating power ratio

8. Third-party projects and Helmholtz projects

Project	Full title	Funded by/ source
HyCavMobil	Hydrogen Cavern for Mobility – Untersuchung von Salzkavernen als potenziellen Speicherort für Wasserstoff	Bundesministerium für Verkehr und digitale Infrastruktur (BMVI) im NIP II (Nationales Innovationsprogramm Wasserstoff- und Brennstoffzellentechnologie) mit NOW GmbH (Nationale Organisation Wasserstoff- und Brennstoffzellentechnologie) als Koordinator
HyTazer	Hydrogen Tank Zertifizierung	Helmholtz Association of German Research Centers
H2Cast-Ready		Mittel des Landes Niedersachen
H2Cast-Prove	Verbundvorhaben H2CAST-Prove: Untersuchung hochflexibler Betriebsfahrweisen von Salzkavernen und Obertageanlagen zur Wasserstoffspeicherung unter Nutzung von Sole-Pendelung	Bundesministerium für Wirtschaft und Klimaschutz (BMWK)
MuSeKo	MULTI-SEKTOR-KOPPLUNG	Bundesministerium für Wirtschaft und Klimaschutz (BMWE)
HyReK	Hybrid Regel Kraftwerk 2.0 - Entwicklung, Optimierung und Validierung eines sektorenkoppelnden Hybridspeichersystems zur Bereitstellung von Primärregelleistung Teilvorhaben: Modellgestützte Betriebsstrategieoptimierung zum Lastmanagement und dessen multikriterielle Bewertung	Bundesministerium für Wirtschaft und Klimaschutz (BMWK)
UP-TO-ME	Unmanned Power-To-Methanol Production	EU Horizon Europe
BuildHEAT	Standardized approaches and products fort the systemic retrofit of residential Buildings, focusing on HEATing and cooling consumptions attenuation in short BuildHEAT;	EU Horizon 2020
Ever	Energy and Transport	Helmholtz Association of German Research Centers
D2SERVICE	Design of 2 Technologies & Applications to Service	EU, Horizon 2020
LifetimeINH5000	Verbundprojekt: LifetimeINH500: Erforschung von Lösungsansätzen zur Maximierung der Lebensdauer und Effizienz eines 5kW-PEM-Brennstoffzellen-BHKWs	Bundesministerium für Wirtschaft und Energie
LLEC::JuPilot	LLEC::JuPilot -Ein Demonstrator am Schülerlabor JuLab	Federal Ministry of Education and Research (BMBF)

LLEC::KNV	Klimaneutraler Verwaltungsbau als aktiver Teil des Living Lab Energy Campus (LLEC)	Federal Ministry for Economic Affairs and Climate Action (BMWK)
LLEC::PtG++	LLEC::P2G++ Saisonale Speicherung in gekoppelten, regenerativen Energiesystemen mittels Power-to-Gas (P2G)	Federal Ministry of Education and Research (BMBF)
LLEC::SK	LLEC: Living Lab Energy Campus Jülich	Federal Ministry for Economic Affairs and Climate Action (BMWK)
LLEC::VxG	LLEC::VxG – Integration von "Vehicle-to-grid"-Applikationen zur Bereitstellung von Systemdienstleistungen in intelligenten Energienetzen	Federal Ministry of Education and Research (BMBF)
NOVAREF	Erstellung neuer Referenzlastprofile zur Auslegung, Dimensionierung und Wirtschaftlichkeitsberechnung von Hausenergieversorungssystemen	Bundesministerium für Wirtschaft und Energie
SDK2050	Systemdienlichkeit 2050	Helmholtz Association of German Research Centers
HDS-LEE	Helmholtz School for Data Science in Life, Earth and Energy, Helmholtz Association of German Research Centers	Helmholtz Association of German Research Centers
UQ	Helmholtz Incubator Pilot Project "Uncertainty Quantification,", Helmholtz Association of German Research Centers	Helmholtz Association of German Research Centers
UP-TO-ME	Unmanned-Power-to-Methanol-production	EU Horizon Europe

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