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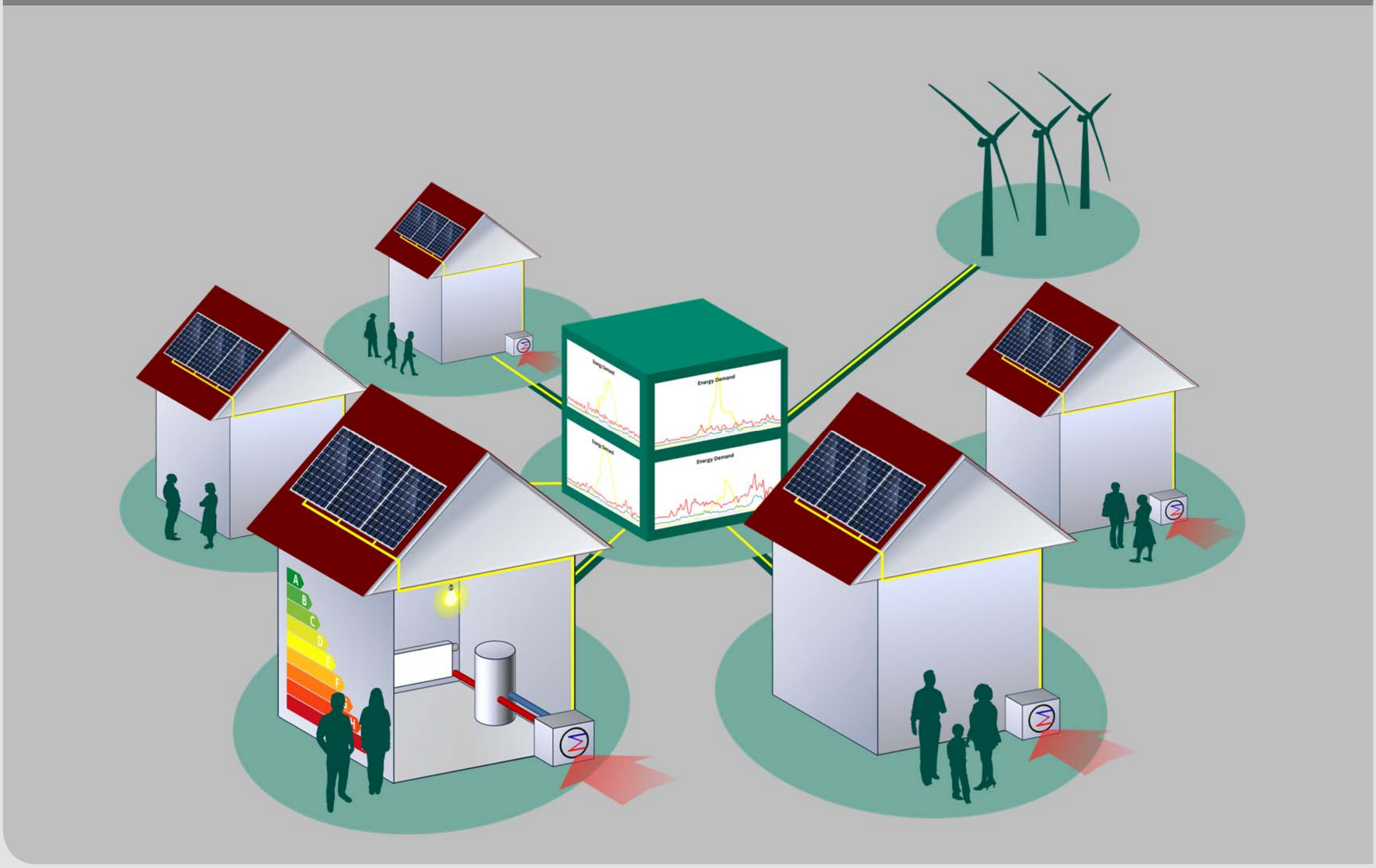

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The trend towards decentralized energy systems with an emphasis on renewable energy sources (RES) causes increased fluctuations and non-negligible weather-related uncertainties on the future supply side. Stochastic modeling techniques enable an adequate consideration of uncertainties in the investment and operation planning process of decentralized energy systems. The challenge is that modeling of real energy systems ends up in large-scale problems, already as deterministic program. In order to keep the stochastic problem feasible, we present a module-based, parallel computing approach using decomposing techniques and a hill-climbing algorithm in combination with high-performance computing (HPC) for a two-stage stochastic optimization problem. Consistent ensembles of the required input data are simulated by a Markov process and transformed into sets of energy demand and supply profiles. The approach is demonstrated for a residential quarter using photovoltaic (PV) systems in combination with heat pumps and storages. Depending on the installed technologies, the quarter is modeled either as stochastic linear program (SLP) or stochastic mixed-integer linear program (SMILP). Our results show that thermal storages in such a decentralized energy system prove beneficial and that they are more profitable for domestic hot water than for space heating. Moreover, the storage capacity for space heating is generally larger when uncertainties are considered in comparison to the deterministic optimization, i.e. stochastic optimization can help to avoid bad layout decisions.

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Abstract

The trend towards decentralized energy systems with an emphasis on renewable energy sources (RES) causes increased fluctuations and non-negligible weather-related uncertainties on the future supply side. Stochastic modeling techniques enable an adequate consideration of uncertainties in the investment and operation planning process of decentralized energy systems. The challenge is that modeling of real energy systems ends up in large-scale problems, already as deterministic program. In order to keep the stochastic problem feasible, we present a module-based, parallel computing approach using decomposing techniques and a hill-climbing algorithm in combination with high-performance computing (HPC) for a two-stage stochastic optimization problem. Consistent ensembles of the required input data are simulated by a Markov process and transformed into sets of energy demand and supply profiles. The approach is demonstrated for a residential quarter using photovoltaic (PV) systems in combination with heat pumps and storages. Depending on the installed technologies, the quarter is modeled either as stochastic linear program (SLP) or stochastic mixed-integer linear program (SMILP). Our results show that thermal storages in such a decentralized energy system prove beneficial and that they are more profitable for domestic hot water than for space heating. Moreover, the storage capacity for space heating is generally larger when uncertainties are considered in comparison to the deterministic optimization, i.e. stochastic optimization can help to avoid bad layout decisions.

1. Introduction

At the current time, our provision of energy is moving from a conventional centralized towards a decentralized energy supply with a significant expansion of renewable energy sources (RES). This fundamental, structural rearrangement of the energy system introduces an increased fluctuation and non-negligible uncertainties on the future supply side. The resulting challenge is the actual technical and economical realization of the transition process. The challenging task is also modeling such energy systems taking into account their uncertainties to support a reliable, cost-efficient and technically feasible transition. In this context, energy systems with decentralized energy provision and load shift potentials by integrated, intelligent home energy management applications or energy storages are becoming increasingly important. The research need is to develop an approach for determining optimal dimension and usage of the decentralized energy system's components, i.e. to support long-term investment and short-term operation decisions under uncertain conditions.

In this paper, we model a residential quarter with photovoltaic (PV) generators and load flexibilities using heat pumps in combination with thermal storages based on a general framework. Our target is to support the investment and operation process of the quarter's energy system. The calculations are based on real data for a new residential quarter located in Germany.

a. Problem setting and related work

Numerous decentralized as well as national and international centralized energy system models are designed for a specific system describing the interaction between energy suppliers, consumers and storages (for a thorough overview see, e.g., Ventosa, Baíllo, Ramos, and Rivier (2005) or Connolly, Lund, Mathiesen, and Leahy (2010)). Depending on the scope of time, the majority is based on time slices from 10 up to 35040 slices per year, which already leads to large-scale problems when realistic energy systems are considered (e.g., see Jochem, Schönfelder, and Fichtner (2015) who need to consider the optimal operation of micro combined heat and power (micro-CHP) units in households in a temporal resolution of 15 minutes to model the physical system properties adequately). Here, the term 'large-scale' does not refer to the geographic size of such a system, but to the number of decision variables which contours the complexity of the optimization model. According to Ventosa, Baíllo, Ramos, and Rivier (2005), large-scale problems have more than $10\,000$ variables and their computational expenses are already high.

The economic profitability of energy systems principally depends on optimal energy management, i.e. on finding the optimal capacity of individual components at the first stage and, at the second stage, on their optimal operation over their lifetimes. The energy management and thus the economic profitability are subject to manifold uncertainties, associated with the future development of electricity prices, the electrical and thermal demand and the energy supply. This is especially true, given that the determined capacities should be optimized over at least a 20-year period. In practice, the impact of uncertainties is often considered by using average values or estimated by sensitivity or scenario analyses since the variation of parameters by such analyses does not increase the problem size. However, such analyses can only provide an estimation of the effect on the optimization results, but the complex impact cannot be captured entirely. Stochastic modeling techniques enable an adequate consideration of various uncertainties in the investment and the operation planning processes, thus supporting the assessment of the system's performance in both the short-term and long-term. There are several individual models for real energy systems that support optimal investment and operation decisions and allow for taking into account uncertainties by stochastic programs (SP) (see for example Möst and Keles (2010), Wallace and Fleten (2003), Kelman, Barroso, and Pereira (2001) and Göbelt (2001)). Most of them deal with continuous or mixed-integer decision variables and linear objective functions and constraints. But there is a gap of a general approach with a comprehensive modeling chain that generates the required energy profiles under consideration of their mutual dependencies and which are used for the resulting large-scale SP with millions of variables to take into account the uncertain conditions.

b. Methodological approach of the case study

As conceptual framework, we present a module-based approach for (a) simulating consistent ensembles of the required input data by a stochastic process, (b) transforming these initial profiles into consistent sets of energy supply and demand profiles and (c) using the generated profiles in a two-stage SP optimization. Since RES supply, such as PV generation, and energy demand depend essentially on fluctuating and uncertain meteorological data, a Markov process is used to generate profiles of the required meteorological parameters considering their stochastic nature. As mentioned above, our focus is not only on operation, but also on investment optimization. Therefore, our approach needs to take into account the short-term (intra-daily) and long-term (annual and seasonal) variations, since both can affect the optimal investment decision. The resulting meteorological profiles are transformed into PV supply and energy demand profiles for the subsequent optimization of the stochastic program. Depending on the different installed technologies, the quarter is modeled either as a stochastic linear program (SLP) or a stochastic mixed-integer linear program (SMILP) ending up in an extreme large-scale energy system model with more than 100 million variables. Besides analyzing the dimensions and usage of the system's components, the optimization model can be used, for instance, to evaluate the impact of different tariffs or to compare other technologies, e.g., wind turbines on the supply side or electrical storages as load shifting units. In general, the framework serves as modeling and optimizing concept for a wide variety of decentralized energy systems with various energy supply and demand components, all under consideration of uncertain conditions. Making use of SP instead of deterministic programming leads to the expected best solution with respect to the uncertainties. The resulting large-scale stochastic problem is decomposed into numerous subproblems and computed in parallel on high-performance computing (HPC) systems to keep the problem feasible. A commercial solver is used for the inner optimization of the subproblems. The entire problem is heuristically solved by a hill-climbing algorithm that coordinates the optimization of the outer masterproblem on the HPC system within an acceptable period of time.

The theoretical background is summarized in section 2 and the approach itself is described in section 3. The focus of the paper is on the presentation of a real-world case study in section 4. In this context, we demonstrate our approach for a residential quarter including approx. 70 households, a 240kWp PV system and heat pumps and heat storages to cover the energy demand. Subsequently, the results are discussed at the end of section 4 and the approach is separately discussed in section 5. The paper finishes with a conclusion and an outlook.

2. Theoretical background – two-stage stochastic programming

Two-stage stochastic programming enables an adequate consideration of different sources of uncertainties in the investment and operation planning process of decentralized energy systems. Generally, uncertainties can be defined as information not exactly known (or neglected) at the time when the decision has to be made. There are manifold ways to classify uncertainties; they can be generally categorized as either aleatory or epistemic (see e.g., Goldstein (2012), Mustajoki, Hämäläinen, and Lindstedt (2006), Bedford and Cooke (2001), French (1995) as well as Morgen and Henrion (1992)).[1] In our context, model results are subject to three different sources of uncertainties:

- (Raw) Input data
- Preparatory transformation of the (raw) input data
- System modelling

Each optimization model requires input data, for example weather, prices, supply or demand categorizable as aleatory, fraught with uncertainties. Additional aleatory or epistemic

[1] Uncertainties are characterized as epistemic, if there is a possibility to reduce them by gathering more data or by refining models. They are aleatory, if the modeler does not foresee the possibility of reducing them (Kiureghian & Ditlevsen, 2007).

uncertainties are introduced by the transformation process of input data to data required for the optimization. (For example, further uncertainties are attached by transforming weather data into electricity supply of renewable energies like wind or PV). Finally, uncertainties are induced by the model itself, mostly epistemically: the more it differs from the real system the more uncertainty could be induced. The optimization results and the consequent decision depend on all these sources of uncertainties. Stochastic modeling techniques can be used to account for the associated uncertainties of input and transformed data, resulting in a robust-sufficient solution that is expectedly optimal.

An optimization under uncertainties has been initially considered about 60 years ago by Dantzig (1955) and by Beale (1955), where values of model parameters were considered as not exactly known. Those parameter uncertainties are incorporated by their probability distributions through stochastic programming (SP).[2] Since economic profitability of an energy system depends predominantly, at the first stage, on the investment decision and, at the second stage, on its operation, the problem can be adequately formulated as a two-stage stochastic program with recourse (Dantzig & Infanger, 2011; Kalvelagen, 2003):

$$\begin{aligned} \min_{x} \quad & c^T x + E_\omega Q(x,\omega) \\ s.t. \quad & Ax = b, \\ & x \geq 0, \end{aligned} \tag{1}$$

where

$$\begin{aligned} \mathrm{Q}(\mathrm{x},\omega) := \; & \min_{y} q_\omega^T y \\ s.t. \quad & T_\omega x + W_\omega y \leq d_\omega \\ & y \geq 0. \end{aligned} \tag{2}$$

The first stage is expressed by (1) with the (first-stage) vector x of the decision variables. The objective function coefficients c^T, the matrix of constraint coefficients A and the right-hand side vector b of the first stage are assumed to be known with certainty. The expectation E of the second-stage objective function Q, a product of the (second-stage) decision variables of y and the objective function coefficients q, is restricted by the transition matrix T and the first-stage variables of x, the technology matrix W and the right-hand side vector d. Because T, W, d and q are not known with certainty, ω denotes a possible scenario with respect to the probability space (Ω, P).

Two-stage SLP without integer requirements in (2) are well-studied (Schultz, 2003). In this case, Q is a piecewise linear convex function. A number of algorithms have been developed for that problem classes (see Ruszczynski (1999)). Most of these algorithms use an extension of the Benders decomposition introduced by Van Slyke and Wets (1969) which in the case of SP is known as the L-shaped method. But for many cases, some decisions of the first and second stage can only be made on the basis of a stepwise selection. Then the main challenge arises when integer variables have to be involved and the convexity is not present anymore (Schultz (2003), see also Haneveld and Vlerk (1999) for some major results in the area).

Birge and Louveaux (1997) have shown a branch-and-cut approach with the L-shaped method for the simplest form of two-stage stochastic integer programs: first-stage purely

[2] At about the same time, the principle of robust optimization was introduced by Wald, A. (1945) next to stochastic programming. It is an alternative approach to counteract uncertainties by minimizing the maximum risk, later termed as optimizing the worst case (Ben-Tal, Ghaoui, & Nemirovski, 2009). Furthermore, fuzzy or parametric programming can be used as other opportunities to incorporate such uncertainties into the optimization model (see Zhou (1998), Verderame, Elia, Li, and Floudas, (2010) and Metaxiotis, K. (2010)).

binary and second-stage continuous variables. For the most challenging class, having integer and continuous variables in both stages and the uncertain parameter can appear anywhere in the model, only few algorithms can be quoted in the existing literature. When integer variables are involved in the second stage, the L-shaped method (that requires convex subproblem value functions) cannot be directly applied. See Escudero, Garín, Merino, and Pérez (2010a) for a thorough review of this subject.

Carøe and Tind (1998) and Carøe and Schultz (1999) presented a generalized L-shaped method for models having integer variables on the second stage and either some continuous or some discrete first-stage variables. The dual-decomposition-based method focuses on using Lagrangian relaxation to obtain appropriate bounds. For large number of mixed-integer variables in both stages, Nurnberg and Römisch (2002) have used stochastic dynamic programming (SDP) techniques. Sherali and Fraticelli (2002), Sen and Sherali (2006) and Zhu (2006) have developed a branch-and-cut decomposition by modifying the L-shaped method by a relaxation in combination with a special convexification scheme called reformulation-linearization technique (RLT). Yuan and Sen (2009) and Sherali and Smith (2009) have enhanced this approach using Benders decomposition on the first stage and a stochastic branch-and-cut algorithm on the second. Alonso-Ayuso, Escudero, and Ortuño (2003) have introduced a branch-and-fix coordination (BFC) methodology with the main difference to the common branch-and-bound algorithm that the search tree evaluates many subproblems and the decision to branch, prune or bound depends on all these subproblems at each step. This approach has been continually upgraded up to using the twin node family (TNF) concept in combination with Benders decomposition schemes (to solve a given relaxed program at each TNF integer set) and parallel processing for continuous and binary variables in both stages (Alonso-Ayuso, Escudero, Garín, Ortuño, & Pérez, 2005; Escudero, Garín, Merino, & Pérez, 2007, 2010a, 2010b, 2012; Pagès-Bernaus, Pérez-Valdés, & Tomasgarda, 2015).

Besides these exact algorithms for solving SMILP, there are also heuristic approaches: For instance, Till, Sand, Urselmann, and Engell (2007) propose a hybrid algorithm that is similar to our approach. It solves two-stage stochastic integer programs with integer and continuous variables in any stage. Based on stage-decomposition, the decomposed second-stage scenario problems are solved by a MILP solver. An evolutionary algorithm performs the search of the first-stage variables. This procedure as well as exact algorithms is not practically applicable for extremely large-scale problems due the high computational expenses of each iteration step. In contrast, we present a module-based approach where a well-performing, hill-climbing algorithm finds an optimal solution of the first-stage variables in few steps. Furthermore, a necessary decomposition of the second stage is applied to achieve solutions with an acceptable accuracy within an acceptable period of time. Because of the extreme problem size, the decomposed second stage is computed in parallel.

3. The developed approach for two-stage stochastic, large-scale problems

In practice, an approach is needed for the economic optimization of decentralized energy systems under uncertainties, such as a residential quarter with storages and its own PV energy provision. To support the investment and operation decisions, the problem is formulated as stochastic program. In the context of a decentralized energy system, optimal decisions are achieved by an optimal consolidation of its energy supply and demand with the objective of, for instance, maximal profits or minimal costs. Furthermore, the objective can depend on parameters as prices, efficiencies and many others. Some of these cannot be used directly for the optimization, but have to be derived from raw data that are transformed into the required format for the optimization. As the entire model chain is subject to the different uncertainties mentioned above, we propose a comprehensive approach that is structured into three subsystems (see Fig.1):

a) Input data subsystem (IDS)
b) Data transformation subsystem (DTS)
c) Economic optimization subsystem (EOS)

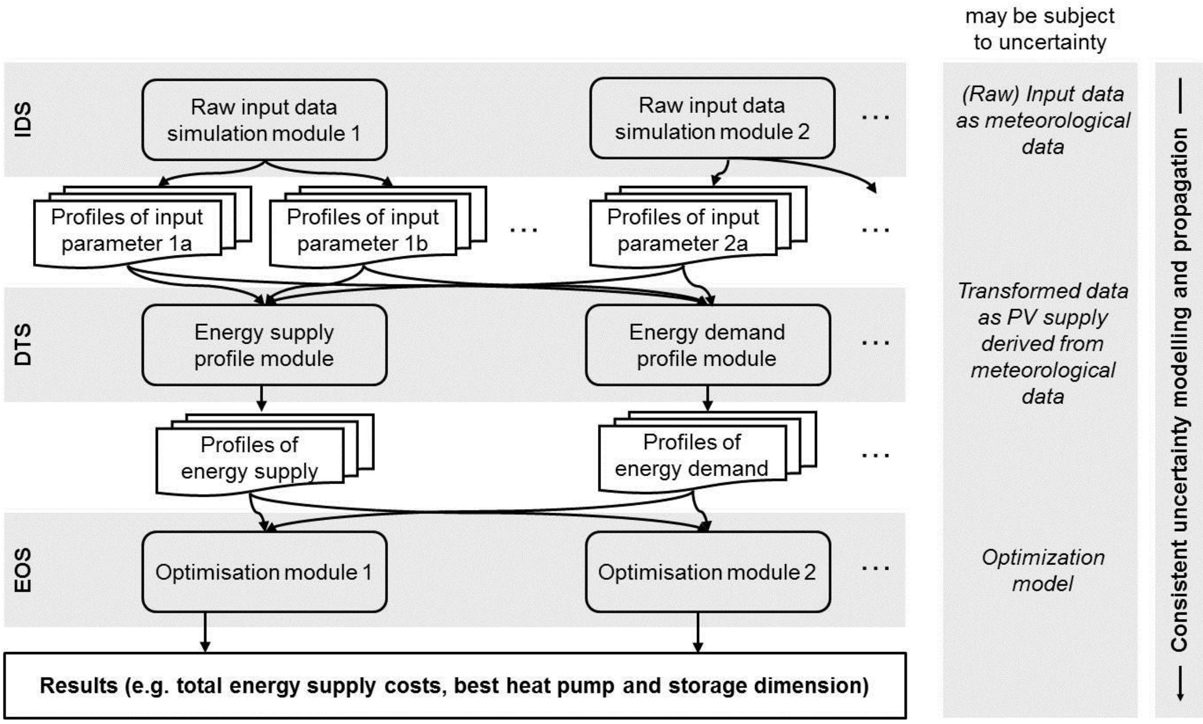


Fig.1: *Conceptual structure of the developed comprehensive modeling approach (Bertsch, Schwarz, & Fichtner, 2014).*

For the optimization of the energy system, data of energy demand, supply and prices are needed which can be either directly acquired as input data or are deduced from raw input data by the DTS. The approach accounts for the associated uncertainties by generating consistent ensembles of raw input parameters (e.g. weather, prices) and transformed data (e.g. electrical and thermal supply or demand) in dependency of their probabilistic properties, i.e. it includes the fundamental relationships between these input parameters and energy demand as well as supply. These profiles are used in the subsequent optimization.

a. Input data subsystem (IDS)

The main task of the IDS consists in generating input parameter profiles (e.g., meteorological profiles, such as global solar radiation and temperature) considering their fluctuating and stochastic nature as well as the interdependencies between them. Our ultimate target in this paper is the two-stage optimization of decentralized energy systems. On the one hand, this implies that our approach for simulating input profiles needs to take into account both, the short-term fluctuations and uncertainties of the different load profiles as well as the long-term variations, e.g., ‘good’ and ‘bad’ solar years, since both variations may affect the choice of adequate dimensions for the components of a decentralized energy system. On the other hand, the decentralized energy system includes components on the supply and the demand side. Therefore, our approach needs to be able to consider the interdependencies between the supply and demand profiles and the meteorological conditions, i.e. an independent stochastic simulation of the profiles would not be appropriate. For instance, the electricity generation from solar PV panels does not only depend on the global solar radiation but also on the temperature, which affects the panels' efficiency. Moreover, the heat demand depends on the temperature as well as the cloudiness. We therefore need to simulate the meteorological conditions, such as the cloudiness, and its interdependencies with temperature and global solar radiation.

The stochastic characterization of solar radiation and other meteorological parameters has been studied intensely in literature. The approaches can generally be divided into two categories: First, regression based models draw random variables applying an estimate of the probability distribution functions of the observations (see Diagne et al. (2013) for an overview for instance). Second, Markov processes draw a random variable applying a transition matrix which represents the probabilities of future states depending on past realizations. For instance, focussing on the long-term variations, Amato et al. (1986) model daily solar radiation using a Markov process. Ehnberg and Bollen (2005) simulate solar radiation on the basis of cloud observations available in three-hour intervals. Focussing on the short-term variations in a high temporal resolution, Morf (1998) proposes a Markov process aimed at simulating the dynamic behaviour of solar radiation.

Overall, Markov processes have proven suitable to meet the above-mentioned requirements, e.g., to consider interdependencies between cloudiness, temperature and global solar radiation. While our approach is similar to the one by Ehnberg and Bollen (2005), we additionally include seasonal information in our Markov process, i.e. the corresponding transition probabilities may vary from month to month (see below). Moreover, we simulate temperature profiles, which are consistently compatible with the simulated radiation profiles.

In order to address the challenge of considering long-term as well as short-term variations, we suggest a two-step approach. In the first step, we start by modeling the daily cloudiness index $\zeta \in \{0, \dots, 8\}$ as a Markov process in order to take the long-term variations into account. The cloudiness is considered in Oktas, describing how many eighths of the sky are covered by clouds, i.e. $\zeta = 0$ indicates a completely clear sky while $\zeta = 8$ indicates a completely clouded sky (Jones, 1992). The following transition matrix is defined for the Markov process used for simulation the cloudiness ζ:

$$\Theta_{\zeta}^{m} = \begin{pmatrix} \pi_{00}^{\zeta,m} & \dots & \pi_{08}^{\zeta,m} \\ \vdots & \ddots & \vdots \\ \pi_{80}^{\zeta,m} & \dots & \pi_{88}^{\zeta,m} \end{pmatrix}. \tag{3}$$

The transition probabilities $\pi_{ij}^{\zeta,m}$ in equation (3) are derived on the basis of publicly available weather data provided by Germany's National Meteorological Service ('Deutscher Wetterdienst (DWD)'), which are available for a variety of locations across Germany for periods of often more than 50 years. A transition probability $\pi_{ij}^{\zeta,m}$ denotes the conditional probability that, in month m, the cloudiness ζ on day δ equals j knowing that the cloudiness on day $\delta - 1$ was i:

$$\pi_{ij}^{\zeta,m} = P(\zeta_{\delta} = j \mid \zeta_{\delta-1} = i); \; \sum_{j} \pi_{ij}^{\zeta,m} = 1 \;\; \forall m \, \forall i. \tag{4}$$

An additional Markov process is used for modeling the daily global solar radiation on the basis of the cloudiness. The transition probabilities of the transition matrix $\Theta_{\rho}^{m,\zeta}$ corresponding to the daily global solar radiation ρ_{δ} on day δ can be expressed as a function of the month m, the cloudiness ζ_{δ} on day δ and the global solar radiation $\rho_{\delta-1}$ on day $\delta - 1$:

$$\pi_{kl}^{\rho,m,j} = P(\rho_{\delta} = l \mid \rho_{\delta-1} = k \cap \zeta_{\delta} = j); \sum_{l} \pi_{kl}^{\rho,m,j} = 1 \;\; \forall m \, \forall j \, \forall k. \qquad (5)$$

The starting values of the Markov processes can be chosen arbitrarily since the influence is negligible in the long run. On the basis of the simulated daily cloudiness, the values for daily global solar radiation and average daily temperature are derived. Our analysis shows that deriving the transition probabilities on a monthly basis delivers more accurate results than using yearly transition probabilities. Overall, a backtesting of our simulation approach shows satisfying results, not only concerning the bandwidth and distribution (e.g., of the average yearly cloudiness) but also concerning the volatility (e.g., of the daily cloudiness values).

In the second step, a stochastic process is used to generate hourly profiles on the basis of the daily simulation results of step 1. This second step accounts for the short-term fluctuations. While in general, the seasonal and daily variations of global solar radiation, for instance, can be described in a deterministic way, the stochastic short-term variations are related to the state of the atmosphere (e.g. the cloudiness). These short-term variations are simulated by an empirically determined, statistically varying term under the constraint that a given daily global solar radiation (determined in step 1) is achieved. The Markov process generates time series of the required input parameters for the following subsystems and is applied to obtain the desired number of scenarios $\omega \in \{1 \dots N\}$ that are the basis of the case study in section 4.

b. Data transformation subsystem (DTS)

The DTS transforms the output of the IDS into data required for the subsequent optimization: energy supply and demand profiles of the decentralized energy system. A PV supply profile module provides the energy supply profiles of the PV system taking into account the physical relationships. Main components of a PV system are solar modules which transform light into electrical energy by the photovoltaic effect. Their electrical energy yield primarily depends on incident light, module efficiency and its orientation described by longitude, latitude, tilt and azimuth of the module. This dependency is formulated by a physical model on the basis of Ritzenhoff (2006). The global solar radiation coming from the IDS is split into direct and diffuse solar radiation on the module and is used as well as ambient temperature to determine accurate module efficiency.[3] Outputs are electrical energy supply profiles for the EOS. Concerning the energy demand, we use a reference load profile approach in the DTS. The generation of heat demand profiles for space heating (SH) and domestic hot water (DHW) is based on the VDI guideline 4655 (2006), using parameters such as season, temperature, cloudiness, insulation, location and occupancy. To generate

[3] The model also includes the albedo effect, averaged losses like shadowing, module miss matching cable or inverter losses for a certain PV system and the dependency of performance on low lighting and temperature for a certain module technology and manufacturer.

electricity demand profiles, the DTS process uses the so-called 'standard load' or H0 profile.[4] Figure 2 illustrates energy demand and supply profiles of a residential quarter having a PV system and energy need of 70 households for electricity, SH and DHW. The electricity can also be taken from an external supplier, while heat demand is covered by heat pumps, heating elements and heat storages within the quarter.

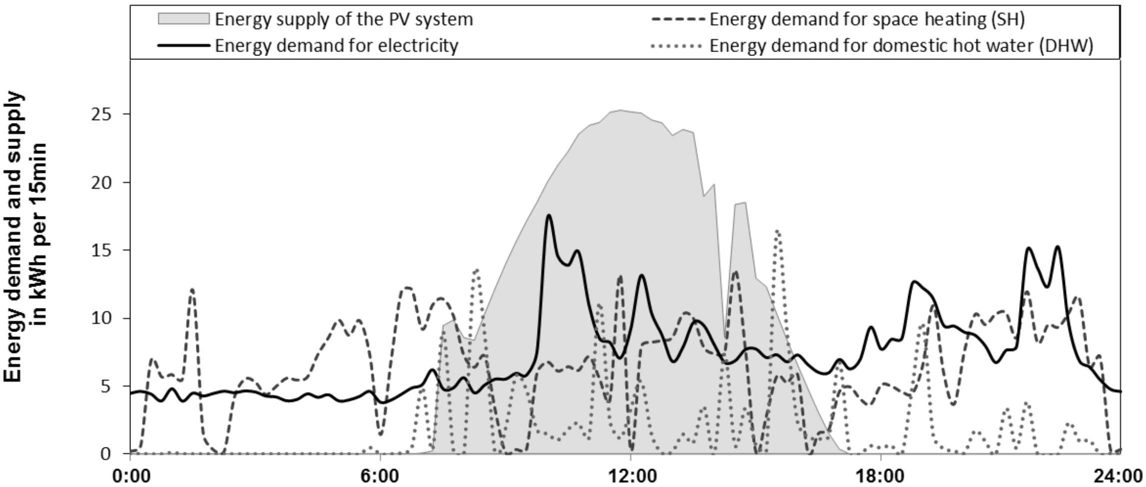


***Fig.2**: Illustrative energy demand and PV supply profiles of a residential quarter for a typical day.*

With respect to Fig.2, the optimization task is to shift the energy demand for SH (dashed line) and DHW (dotted line) to times when a PV surplus is available or energy costs from the grid are low by using heat pumps in combination with heat storages. In addition, minimization of storage losses and ramp-up losses of the heat pumps as well as avoiding the use of the inefficient heating elements will lower the energy costs.

c. Economic optimization subsystem (EOS)

Within the EOS, the problem is formulated as SLP or SMILP by different optimization modules tailored to the specific needs of the problem that allow for carrying out optimal economic decisions. Hereby the profiles of the DTS can be used as possible scenarios with the probability of occurrence p. The stochastic program is decomposed into feasible and manageable subproblems. In order to keep the computation time acceptable, the optimization of the decomposed subproblems is executed in parallel on HPC systems, referred to as inner optimization. Within the masterproblem that is referred to as outer optimization, the first-stage variables are optimized by a hill-climbing algorithm.

i. Mathematical modeling of the optimization problem

Generally, finding economic optimal investment and operation decisions under uncertain parameters can be formulated as a two-stage stochastic program on the basis of equations (1) and (2). Their analytical solution, however, is only possible for few simple cases. In order to solve the two-stage stochastic problem numerically, it can be formulated as one large

[4] Our analysis has shown a strong convergence of aggregate household load towards the H0 profile even for numbers of households much lower than 70.

linear program known as its deterministic equivalent (Dantzig & Infanger, 2011; Ruszczyński & Świętanowski, 1977):

$$\min_{x,y_\omega} \quad c^T x + p_1 q_1^T y_1 + \cdots + p_\omega q_\omega^T y_\omega + \cdots + p_N q_N^T y_N \tag{6}$$

$$s.t. \quad Ax \le b, \tag{7}$$

$$\begin{array}{lllll} T_1 x + W_1 y_1 & & & & \le h_1, \\ \vdots & \ddots & & & \vdots \\ T_\omega x & & + W_\omega y_\omega & & \le h_\omega, \\ \vdots & & & \ddots & \vdots \\ T_N x & & & + W_N y_N & \le h_{\omega,} \end{array} \tag{8}$$

$$x, \quad y_1 \quad \cdots \quad y_\omega, \quad \cdots \quad y_N \quad \ge 0. \tag{9}$$

Hereby, each scenario ω is element of the set of scenarios $\Omega = \{1,2,\ldots,N\}$ occurring with probabilities $p_1,\ldots,p_N$, respectively.[5] In case of mixed-integer decision variables, x and y are defined as (Ahmed, 2011):

$$x \in \mathbb{R}_+^{k_1-l_1} \times \mathbb{Z}_+^{l_1}, \qquad y \in \mathbb{R}_+^{k_2-l_2} \times \mathbb{Z}_+^{l_2}. \tag{10}$$

where k_1, k_2, l_1 and l_2 are non-negative integers with $l_1 \le k_1$ and $l_2 \le k_2$.

The scenarios have to be generated adequately in dependency of the probability distribution of the uncertain parameters. In the case of stochastic programs with integer recourse, Schultz (1995) has shown that, under mild conditions, discrete distributions can effectively approximate continuous ones to any given accuracy. If all scenarios, derived from historical data of N observations or generated by Monte Carlo sampling techniques, have the same probability of occurrence $\frac{1}{N}$, then the expected value of the objective function of (6) can be estimated by:

$$\min_{x,y_\omega} \quad c^T x + \frac{1}{N}\sum_{\omega=1}^{N} q_\omega^T y_\omega, \tag{11}$$

leading to the so-called sample average approximation (SAA) of the problem (Shapiro, Dentcheva, & Ruszczyński, 2009). By the law of large numbers, the approximated expectation converges pointwise to the exact value as $N \to \infty$ assuming that each scenario is independent of other scenarios.

ii. Decomposition and inner parallel optimization

Because of the extreme problem size, most problems have to be decomposed to keep the stochastic program feasible. In principle, each program can be decomposed when knowing the connecting constraints within and between scenarios. Variables between the scenarios are connected by the so-called non-anticipativity constraint: The decisions has to be made on the first stage, like PV, storage or heat pump investments, without anticipating the actual realization of the scenario on the second stage and has thus hold for all possible scenarios.[6] Relaxing of the non-anticipativity constraint leads to the scenario-wise decomposition. On the

[5] In usual practical applications W and q^T do not depend on ω.

[6] When the stage-variable formulation of equation (1) and (2) is transformed into the scenario-variable formulation where the decision vector x is an result for each scenario ω, then the non-anticipativity constraint $x_1 = \ldots = x_\omega$ emerges.

other hand, a stage-wise decomposition, like the L-shaped method, results in a relaxation of the second-stage constraints that contain first-stage variables. Similar to the approach of Till et al. (2007), we do not relax, but fix those connected variables to decompose the stochastic program without violating the model constraints. Therefore, equation (11) is written in its implicit form as a function of the first-stage decisions:

(Master):
$$\min_{x} \quad f(x) = c^T x + \frac{1}{N}\sum_{\omega=1}^{N} Q_\omega(x) \qquad s.t. \quad Ax \leq b, \tag{12}$$

and for a given x, the evaluation of the implicit second-stage value function $Q_\omega(x)$ requires the solution of N independent subproblems:

(Sub):
$$Q_\omega(x) = \min_{y_\omega} q_\omega^T y_\omega \qquad s.t. \quad T_\omega x + W_\omega y_\omega \leq h_\omega \quad \forall \omega = 1, \dots, N. \tag{13}$$

If necessary, the second stage itself can also be decomposed in M subproblems by determining the ties within the scenario. In energy systems, those are mostly the investments (first-stage decisions) and variables that are linked over time steps like the storage level or losses.

The large-scale stochastic program is decomposed between and within the scenarios into MxN mixed-integer subproblems by fixing their connected variables. Each decomposed second-stage subproblem sp_{mn} is solved by the standard MILP solver CPLEX 12 with a relative gap $< 1\%$. The optimization is executed in parallel using HPC nodes to reduce the computation time. The process is designed to solve the subproblems not only on one, but on computing nodes of different HPC systems. After the optimization of the subproblems, their solution is composed to calculate the minimal value of $f(x)$ for the specific fixed variables x_i. An outer hill-climbing optimization performs the search on the first stage variables. Fig.3 depicts the whole optimization process.

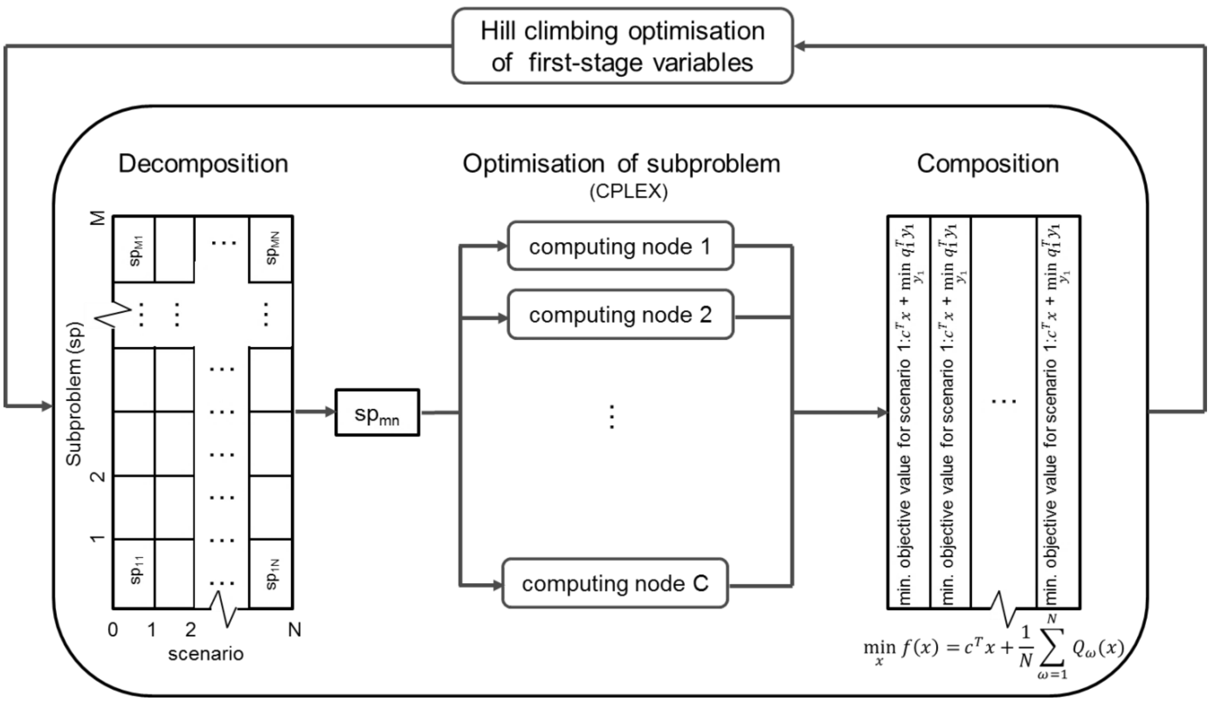


***Fig.3**: Parallel optimization process (POP) for large-scale, two-stage stochastic programs.*

iii. Outer hill-climbing optimization

A hill-climbing algorithm is a local optimization approach that attempts to improve a given initial solution to a problem by incrementally altering its solution-dependent variables (Taborda, & Zdravkovic, 2012). In the optimization process, a steepest-ascent hill-climbing (SAHC) method attempts to minimize the objective function $f(x)$ by adjusting a single element of the first-stage vector x representing an investment as continuous and/or discrete value x_i. Standardly, all components of x are sequentially modified in the direction that improves the value of $f(x)$ at each iteration. The one leading to the greatest increase is accepted (see for example Forrest, S., & Mitchell, M. (1993)). We adapt the steepest-ascent search to reduce the risk of overstepping the global optimum: At each iteration, each first-stage variable x_i, is increased and decreased sequentially by a certain step size s_i. Then the minimal objective values of $f(x \pm s_i e_i)$ are computed by the parallel optimization process (POP) as shown in Fig.3. In this way, the hill-climbing approach can start at any initial solution without knowing the ascending direction beforehand. The step with the best improvement is accepted and the adapted steepest-ascent search is repeated. When there is no improvement, then the step size is divided in half. The process continues until the relative change of $f(x)$ is smaller than a given stopping criterion $a \in \mathbb{R}_+$. The whole procedure is:

Step 0: (**Initialization**) compute $f(x^0)$ for an initial x (e.g. $x = 0$) by using POP and set step size s_i for each investment x_i of vector x. Let $e_i \in \mathbb{R}_+^{k_1}$ be the i-th unit vector.

Step 1a: Add s_i to x_i and compute $f(x + s_i e_i)$ by using POP and subsequently subtract s_i from x_i for each investment $1 \leq x_i \leq k_1$.

Step 1b: Subtract s_i from x_i and compute $f(x - s_i e_i)$ by using POP and subsequently add s_i to x_i for each investment $1 \leq x_i \leq k_1$.

Step 2: Select $x^* \in \{x \pm s_i e_i \mid \forall\, 1 \leq i \leq k_1\}$ with $f(x^*) = \min_i \{f(x \pm s_i e_i)\}$.

Step 3: Define $\Delta f(x)_{rel} = (f(x^0) - f(x^*))/f(x^0)$.

Step 4: If $\Delta f(x)_{rel} \leq 0$, then $s = \frac{s}{2}$ and go to step 1a. Otherwise continue.

Step 5: If $\Delta f(x)_{rel} > a$, then accept $f(x^0) = f(x^*)$ and $x^0 = x^*$ and go to step 1a. Otherwise continue.

Step 6: (**End**) Stop. The local optimal solution value is $f(x^*)$ with the vector x^*.

4. Application of the developed approach to a residential quarter

We demonstrate the described approach for a real-world case study: a residential quarter that is introduced in Section 4a. Its mathematical model and the corresponding computational results are presented in Sections 4b and 4c.

a. Residential quarter

We focus on a residential quarter including 70 households on 7700m^2 in multi-family or row houses that are clustered in several building groups $g \in \{1, \dots, G\}$.[7] Fig.4 shows the energy setup of the quarter that shall be optimized under uncertain conditions.

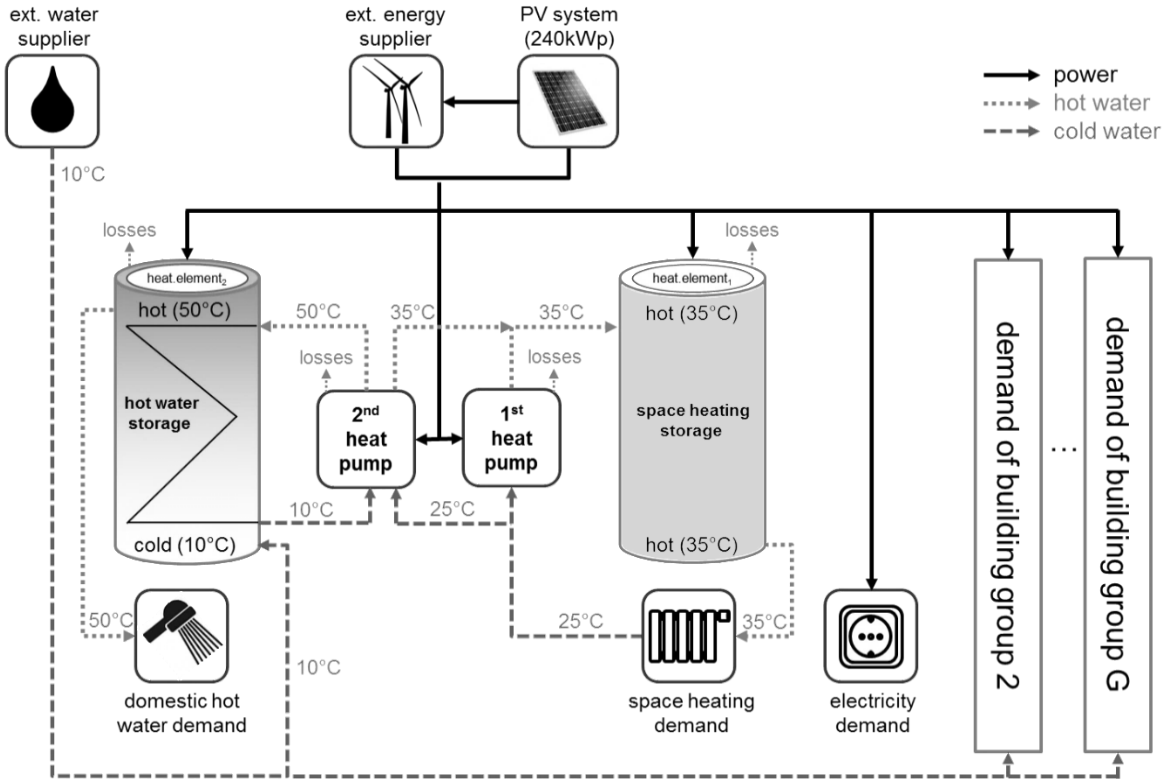


Fig.4: *Energy setup of building group $g \in \{1, \dots, G\}$ of the quarter.*

On the energy supply side, there are a 240kWp PV system and the possibility to obtain electricity, that cannot be covered by own production, from an external energy supplier at an assumed electricity price of $p^{grid} = 0{,}25€/\text{kWh}$. If the PV supply exceeds the electricity demand of the quarter, the surplus can be fed into the external grid by a compensation of $p^{fi} = 0{,}10€/\text{kWh}$. On the energy demand side, there are the electrical and thermal consumption of each building group g. In this case study, the quarter totally consists of $G = 4$ building groups. The thermal consumption, i.e. demand for space heating (SH) and for domestic hot water (DHW), of one building group is covered by two air-water heat pumps in combination with heat storages for each building group. Both heat storages are carried out as hot water tanks having their own electrical heating elements to ensure thermal supply security in times of peak demand and disinfection function. The heating system is separated into two cycles, because it allows the heat pump for SH to run at lower temperatures resulting in a higher coefficient of performance (COP) and lower heat losses of the storage and, thus, in less energy costs. Because of the lower temperatures, underfloor heating systems are installed to exchange the required heat by a larger heat exchanger surface.

[7] The corresponding project is aimed at developing energy-efficient, environmentally friendly residential quarters where a large part of the required energy will be provided by PV systems within the quarters, the energy consumption is reduced by modern passive house technology. An increased PV self-consumption is achieved by heat pumps with storages and intelligent load shifting within the quarter.

SH storages are implemented in a closed cycle and its temperature can be assumed as thoroughly mixed that can drop from $35°C$ up to $10K$. In contrary, due to the fresh water requirements, the loop from the heat pump through DHW storages is separated from the fresh water cycle by a heat exchanger in the tank. The temperature of the fresh water amounts to $10°C$ and needs to heat up to $50°C$.[8] The higher temperature difference results in a larger energy content at the same volume in comparison to SH storages.

The concrete task is to determine optimal storage sizes for SH and DHW of each building group including their optimal operation leading to minimal energy costs. In this case study, two different air-water heat pumps can be installed: one type referred as inverter heat pumps can provide heating power at each level below or equal to their maximum power. The other one, with less investment needs, can only run stepwise at idle, half or full load. Their maximal available heating power and their COP also depend on the ambient air temperature. Further uncertain parameters that vary with weather conditions are PV generation and thermal as well as electrical demand. To determine the economically optimal sizes of the different components and their operation, such as the storage sizes for SH and DHW of each building group, under these uncertain parameters, the energy setup illustrated in Fig.4 is modeled as SLP and SMILP depending on the installed heat pump technology.

b. Mathematical model of the quarter

Corresponding to equation (6), the objective function of the deterministic equivalent for scenario ω that represents the minimization of the total energy costs of the quarter for one possible outcome of Ω can be formulated as:

$$\begin{aligned} costs_{\omega}^{*} = \min_{c_{g,i}, e_{\omega,t}^{grid}, e_{\omega,t}^{fi}} & ANF \sum_{g=1}^{G} \sum_{i=1}^{k_1} cost_i \cdot c_{g,i} \\ & + \sum_{t=1}^{T} e_{\omega,t}^{grid} \cdot p^{grid} - e_{\omega,t}^{fi} \cdot p^{fi}, \end{aligned} \tag{14}$$

where annual capital cost of each investment i of building group g are included by using a discounted cash flow investment evaluation, the equivalent annual cost (EAC) method: Investments are converted into an equivalent series of uniform amounts per period T (Jones, & Smith, 1982).[9] The integrated annuity factor (ANF) takes into account the lifetime of the investment and the possibility that the capital could be invested elsewhere at a certain interest rate. The EAC is often used for investment decisions of (decentralized) energy systems, see for example Silveira and Tuna (2002), Korpaas, Holen, and Hildrum (2003), Hawkes and Leach (2005) or Schicktanz, Wapler, and Henning (2011). In this case study, an interest rate of 10% and a technical lifetime of 20 years is assumed. The period T includes one year with a temporal resolution of 15 minute steps. Further predefined components (in the context of the presented case study) are:

- the installed PV capacity of the quarter: $\sum_{g=1}^{4} c_{g,i=PV} = 240$,

[8] By using the density and heat capacity of water, the volume storage level is converted into an energy storage level required by the optimization model.
[9] The costs for each component $cost_i \cdot c_{g,i}$ are assumed as linear function composed of fix and size-dependent variable investments referring to market prices.

- the number of heat pumps for SH within a building group: $c_{g,i=HP_{SH}} = 1$,
- the number of heat pumps for DHW within a building group: $c_{g,i=HP_{DHW}} = 1$,
- the number of heating elements for the SH storage: $c_{g,i=HE_{SH}} = 4$,
- the number of heating elements for the DHW storage: $c_{g,i=HE_{DHW}} = 4$.

The whole nomenclature is explained in the appendix in Table 1.Technically, the used heating elements can provide heating power continuously below or equal to their maximum power $d^{he,max}$. Similar, the air-water heat pumps, designed as inverter heat pumps, can provide heating power at each level below or equal to their maximum power $d^{hp,max}_{\omega,t}$. The other option is a heat pump that can only run at discrete power output levels. In this case study, the storage size for SH $c_{g,i=S_{SH}}$ and for DHW $c_{g,i=S_{DHW}}$ shall be optimized for inverter heat pumps and for heat pumps that can only run idle, half or full load.

Essential constraints of the system are that the demand and supply need to be balanced at any time:

$$e^{pv}_{\omega,t} + e^{grid}_{\omega,t} = d^{ee}_{\omega,t} + \sum_{g}^{4}\sum_{u=1}^{2}\left(d^{hp}_{\omega,g,u,t} + d^{he}_{\omega,g,u,t}\right) + e^{fi}_{\omega,t} \qquad \forall\omega\ \forall t, \quad (15)$$

$$d^{hp}_{\omega,g,u,t} \cdot COP_{\omega,u,t} + d^{he}_{\omega,g,u,t} \cdot \eta + s_{\omega,g,u,t} = d^{th}_{\omega,g,u,t} + L_{\omega,g,u,t} + s_{\omega,g,u,t+1} \qquad \forall\omega, \forall g, \forall u,\ \forall t. \quad (16)$$

The supplied PV energy depends on the size of the PV system: $e^{pv}_{\omega,t} = \sum_{g=1}^{4} c_{g,i=PV} \cdot e^{pv,kwp}_{\omega,t}$. In equation (16), storage heat losses $L_{\omega,g,u,t}$ are integrated by a constant loss factor l_u in dependency of the heat storage level:

$$L_{\omega,g,u,t} = s_{\omega,g,u,t} \cdot l_u \qquad \forall\omega, \forall g, \forall u,\ \forall t. \quad (17)$$

The storage possibility $s_{\omega,g,u,t}$ is limited by:

$$s^{min}_{g,u} \leq s_{\omega,g,u,t} \leq c_{g,i=S_u} \qquad \forall\omega, \forall g, \forall u,\ \forall t. \quad (18)$$

The heat supply for each building group is limited by the number of heating elements $c_{g,i=HE_u}$ and their maximal power values $d^{he,max}$:

$$d^{he}_{\omega,g,u,t} \cdot \eta \leq c_{g,i=HE_u} \cdot d^{he,max} \qquad \forall\omega, \forall g, \forall u,\ \forall t, \quad (19)$$

and the number of heat pumps $c_{g,i=HP_u}$ and their maximum power values $d^{hp,max}_{t}$:

$$d^{hp}_{\omega,g,u,t} \cdot COP_{\omega,u,t} = z_{\omega,g,u,t} \cdot \frac{1}{m} \cdot d^{hp,max}_{\omega,t} \qquad \forall\omega, \forall g, \forall u, \forall t, \quad (20)$$

$$z_{\omega,g,u=DHW,t} \leq m \cdot c_{g,i=HP_{DHW}} \qquad \forall\omega\ \forall g\ \forall t, \quad (21)$$

$$\sum_{u=1}^{2} z_{\omega,g,u,t} \leq m \cdot \sum_{u=1}^{2} c_{g,i=HP_u} \qquad \forall\omega, \forall g, \forall t. \quad (22)$$

Here, constraints (20)-(22) ensure that both heat pumps can be used to cover the demand for space heating, but only one for domestic hot water. This specific set-up is reasoned by a higher demand for space heating than for domestic hot water (up to ten times on winter days). In case that heat pumps can run only at idle, half or full load, then $m = 2$, representing the possible modes minus the idle mode, and the variables $z_{\omega,g,u.t}$ have to be integers with $z_{\omega,g,u=SH,t} \in \{0,1,2,3,4\}$ and $z_{\omega,g,u=DHW,t} \in \{0,1,2\}$, otherwise continuous variables.

Practically, positive load changes result in higher thermal and mechanical energy consumption of the heat pumps and reduce the COP. Therefore, one further constraint is needed to differentiate linearly between positive and negative load changes of the heat pumps achieved by positive auxiliary variables:

$$z_{\omega,g,u,t+1} - z_{\omega,g,u,t} = pos_{\omega,g,u,t} - neg_{\omega,g,u,t} \qquad \forall\omega, \forall g, \forall u,\ \forall t. \quad (23)$$

To take into account energy losses during positive ramp up times, an additional term $pos_{\omega,g,u,t} \cdot r_u$ is added to the right side of constraint (16) avoiding permanent load changes of the heat pumps. The ramp-up loss of heat pumps is modeled by a loss factor r_u with 5% loss of the positive load change at time t. Additionally, the left side of the constraints (16) can be relaxed by a further auxiliary variable $q_{\omega,g,u,t}$, in the event that heat supply below the demand is acceptable. Then this variable is multiplied by a compensation factor $f = 100\,000€/\mathrm{kWh_{el}}$ and added, as an economic penalty term, to the objective function (14).
For all variables that are connected by a constraint over two time steps, the following constraints equal the element of the first and last time step t:

$$\begin{aligned} s_{\omega,g,u,t=T} &= s_{\omega,g,u,t=1} && \forall\omega, \forall g, \forall u, \\ z_{\omega,g,u,t=T} &= z_{\omega,g,u,t=1} && \forall\omega, \forall g, \forall u. \end{aligned} \quad (24)$$

All presented variables need to be positive. Since the scenarios are generated by a Markov process, the entire stochastic program, minimizing the expected costs, can be solved numerically by adapting (14) analogously to (11):

$$\begin{aligned} costs^* = \min_{c_{g,i}, e^{grid}_{\omega,t}, e^{fi}_{\omega,t}} & ANF \sum_{g=1}^{G} \sum_{i=1}^{k_1} cost_i \cdot c_{g,i} \\ & + \frac{1}{N} \sum_{\omega=1}^{N} \sum_{t=1}^{T} e^{grid}_{\omega,t} \cdot p^{grid} - e^{fi}_{\omega,t} \cdot p^{fi}. \end{aligned} \quad (25)$$

The model dimension of one scenario is shown in Table 2 for one building group and for the entire quarter. In order to allow for an appropriate consideration of the uncertainties, a problem containing hundreds to thousands of such scenarios need to be solved.

Table 2: Model dimension of one scenario ω.

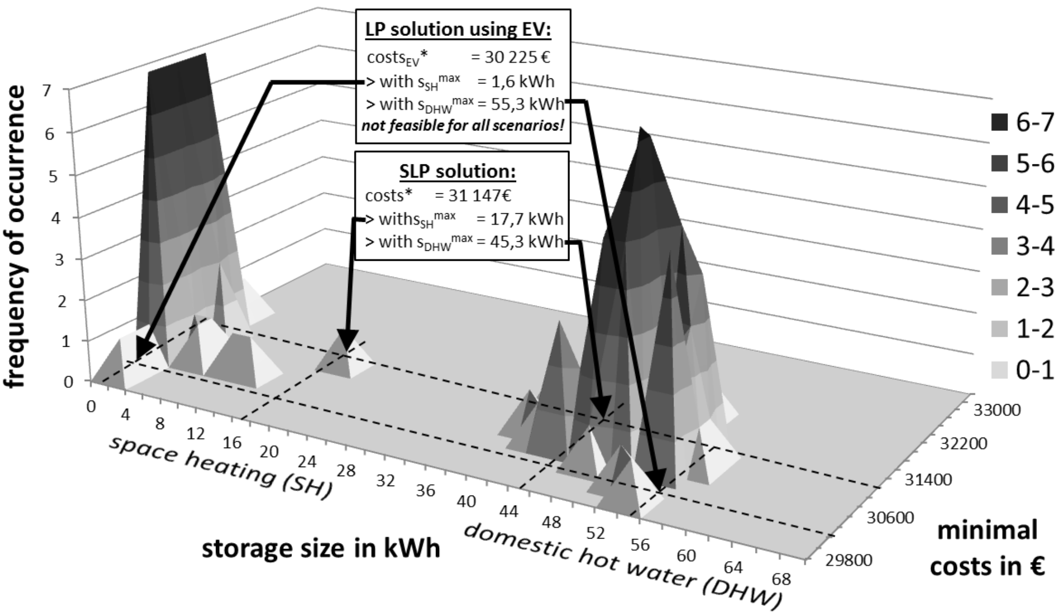
	Continuous variables	Integer variables (continuous if SLP)	Constraints
for building group g	420 486	70 084	946 080
for the entire quarter	1 681 941	280 336	3 048 480

c. Computational results

For this case study, 100 weather scenarios were generated by a Markov process representing the uncertain global solar radiation, temperature and cloudiness. These profiles are transformed into PV supply and energy demand profiles for electricity, SH and DHW that are used in the described SLP and SMILP. According to (12) and (13), equation (25) of the stochastic program is decomposed into 100 subproblems each representing one scenario.

Because of the extreme problem size of one scenario, the one year period T of each scenario is also decomposed into periods of two weeks leading to 27 subproblems per scenario.[10] The resulting 2700 subproblems are solved in parallel by using POP within half an hour. The storage optimization is done for the quarter that is located in Germany. About 20 steps of the outer optimization are needed to find the optimal storage sizes. If the optimization was carried out sequentially on one computer, the computation time would amount to $432\,000$ hours ($about$ 50 years). Due to the POP, the problem is solved within one week. For a better illustration, only the results for building group 1 are presented in the following and subsequently discussed to the end of this paper.

a)



b)

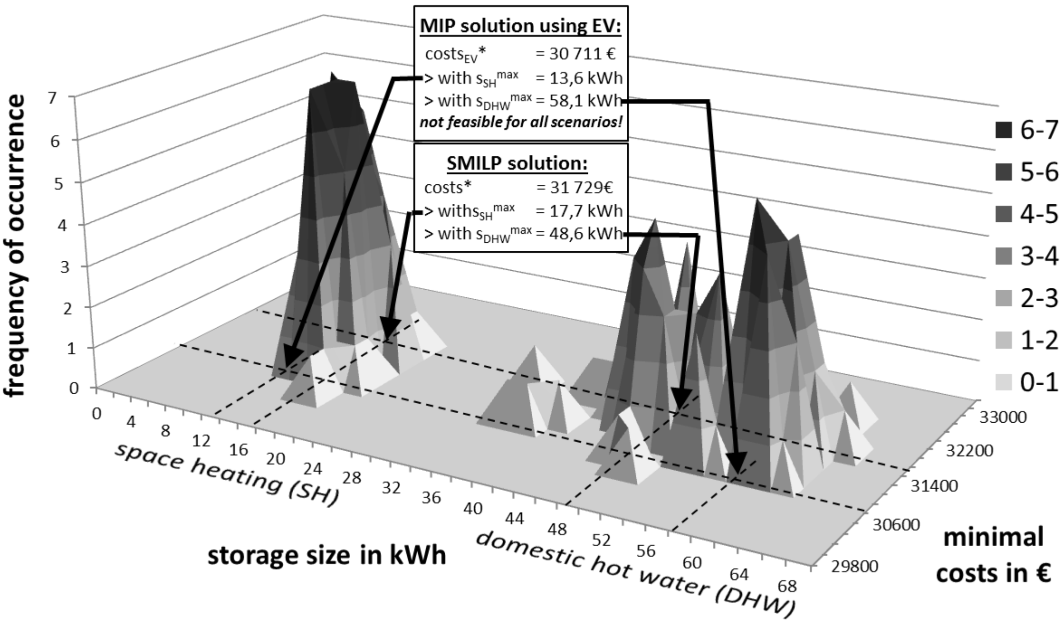


***Fig.5**: Density function of minimal costs and optimal storage size including the stochastic solution and the deterministic solution using expected values of the uncertain parameters of the SLP (a) and SMILP (b) of building group 1.*

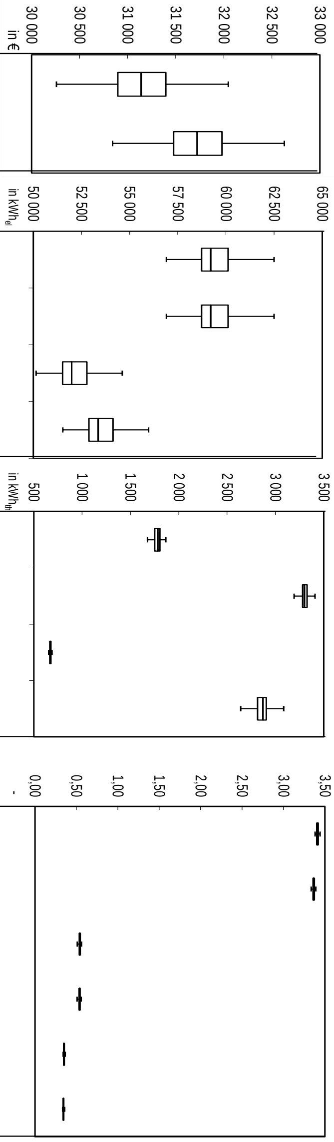
[10] The chosen period of two weeks results in problem size for an efficient utilization of the HPC systems with respect to computation requirements and total computation time.

Fig.5 shows the density function of minimal costs and optimal storage sizes of all scenarios as program with continuous variables (a) or with mixed-integer variables (b) of building group 1. The optimal storage size in $\mathrm{kWh_{th}}$ is plotted on the abscissa (lateral wide axis) for SH ($< 20\mathrm{kWh_{th}}$) and for DHW ($> 30\mathrm{kWh_{th}}$) versus the minimal costs on the ordinate (lateral depth axis) for each scenario independently. The applicate (vertical height axis) contains the information of the frequency of occurrence for the optimal storage size with class intervals of $2\mathrm{kWh_{th}}$ and their according minimal costs within class intervals of $200€$.

When each scenario is optimized separately and inverter heat pumps are in use, i.e. all variables are continuous meaning that the heat pumps can run completely flexibly (Fig.5a), the optimal storage size for SH varies between 1-$17\mathrm{kWh_{th}}$ and for DHW between 40-$55\mathrm{kWh_{th}}$ for building group 1 with 29 households. The frequency peak of occurrence is at the class interval of 0-$2\mathrm{kWh_{th}}$ for SH and of 48-$50\mathrm{kWh_{th}}$ for DHW. The minimal costs amount to $30\,164$ - $31\,957€$ for the SLP. Thereof, approximately 60% can be attributed to the capital costs of the energy system's components. The remaining 40% can be attributed to the variable energy costs. Fig.5 also includes the stochastic solution and the deterministic solution of the expected value problem (EV). The optimal solution of the SLP amounts to $17{,}7\mathrm{kWh_{th}}$ for SH and $45{,}3\ \mathrm{kWh_{th}}$ for DHW with $31\,147€$ minimal expected costs. The solution of the EV is achieved by using expected values of the uncertain input parameters to determistically determine the optimal storage sizes. Then the optimal storage sizes are $1{,}6\mathrm{kWh_{th}}$ and $55{,}3\mathrm{kWh_{th}}$ for SH and DHW, respectively, leading to 3% lower minimal costs.

Fig.5b analogously shows the results for the SMILP. The frequency peak of occurrence is at the class interval of 14-$16\mathrm{kWh_{th}}$ for SH and of 44-$60\mathrm{kWh_{th}}$ for DHW. The optimal solution amounts to $17{,}7\mathrm{kWh_{th}}$ for SH and$48{,}6\mathrm{kWh_{th}}$for DHW. When expected values of the input data are used for the optimization, the storage for SH amounts to $16{,}6\mathrm{kWh_{th}}$ and for DHW to $58{,}1\mathrm{kWh_{th}}$.

quantity (unit)	model	minimum	0.25 quantile	median	0.75 quantile	maximum
minimized costs (in €/a)	SLP	30 258	30 898	31 141	31 398	32 048
	SMILP	30 844	31 478	31 723	31 982	32 629
PV supply* (in kWhel)	SLP	56 914	58 739	59 212	60 116	62 500
$\sum_t e^{pv}_{\omega,t}$	SMILP	56 914	58 739	59 212	60 116	62 500
elect. demand of the heating system (in kWh_{el})	SLP	50 144	51 522	51 994	52 778	54 619
$\sum_t \sum_u (d^{hp}_{\omega,g=1,u,t} + d^{he}_{\omega,g=1,u,t})$	SMILP	51 530	52 888	53 372	54 140	55 984
storage losses (in kWh_{th})	SLP	1 677	1 751	1 783	1 805	1 866
$\sum_t L_{\omega,g,u,t}$	SMILP	3 193	3 282	3 301	3 327	3 410
ramp-up losses (in kWh_{th})	SLP	653	666	670	676	688
$\sum_t \sum_u r_u \cdot pos_{\omega,g=1,u,t}$	SMILP	2 642	2 815	2 870	2 907	3 087
COP** (-)	SLP	3,38	3,40	3,41	3,42	3,44
$\frac{\sum_t \sum_u d^{hp}_{\omega,g=1,u,t}}{\sum_t \sum_u d^{hp}_{\omega,g=1,u,t} \cdot COP_{\omega,u,t}}$	SMILP	3,33	3,36	3,36	3,37	3,39
PV self-consumption (-)	SLP	0,51	0,53	0,54	0,55	0,56
$1 - \left(\frac{\sum_t e^{fi}_{\omega,t}}{\sum_t e^{pv}_{\omega,t}}\right)$	SMILP	0,51	0,53	0,54	0,54	0,56
autarky (-)	SLP	0,34	0,35	0,35	0,35	0,37
$\frac{\sum_t e^{pv}_{\omega,t} - \sum_t e^{fi}_{\omega,t}}{\sum_t \left(d^{ee}_{\omega,t} + \sum_u \left(d^{hp}_{\omega,g=1,u,t} + d^{he}_{\omega,g=1,u,t}\right)\right)}$	SMILP	0,33	0,34	0,34	0,35	0,36



* PV supply is illustratively caclulated for buildiung group 1 in relation of the system area occupied on the building group to the total are of the 240 kWp system.

** COP is calculated for both heat pumps as overall efficiency of provided thermal energy for SH and DHW in relation to demanded elctrical energy of the heat pumps.

Fig.6*: Characteristic values and measures of dispersion of* 100 *scenarios for the optimal solution of SLP and SMILP for building group 1, also shown as box-and-whisker (the whiskers represent the minimum and maximum of the values).*

For the optimal investment solution of the SLP and SMILP, Fig.6 shows variations of characteristic values of the 100 scenarios: minimum, 0.25 quantile, median, 0.75 quantile and maximum of the values are listed as measures of dispersion. Besides, the values are illustrated as box-and-whisker plot rotated through 90°. These values indicate the variations that can be expected when the investment decision is made, i.e. when the first-stage variables are set. The minimum and maximum of the minimized costs for the given optimal storage sizes range between 30 258€ and 32 629€. Note that these values are slightly higher than those of 100 separate (deterministic) optimizations of the storage sizes, in which the first-stage variables are still alterable.

The annual PV supply varies between $56\,914 kWh_{el}$ and $62\,500 kWh_{el}$. The electrical demand of the heating system, the heat pumps and heating elements, amounts to $50\,144\, kWh_{el}$-$54\,619 kWh_{el}$ for the SLP and is approximately $1500 kWh_{el}$ higher for the SMILP.

The higher demand results from different thermal storage losses and ramp-up losses of the heat pumps that are 2-5 times lower when inverter heat pumps are used. The overall COP which is related to the total thermal supply and total electrical demand of both heat pumps is around 3.4 and only marginal better in the case of SLP. Further quantities of interest are the PV self-consumption rate (51-56%) and the actual autarky rate (33-37%). With a marginally varying electricity demand of the households around $40\,000\mathrm{kWh_{el}}$, the annually balanced autarky ranges between 60-70%. Also not listed in Fig.6, the electrical load of the external grid ranges between 39-56kW for the SLP and between 44-57kW for the SMILP.

d. Discussion of the results

The general result is that the usage of thermal storages in such a decentralized energy system with PV supply and energy demand of several households proves beneficial, despite the uncertainties. The DHW storage is larger than the SH storage due to the non-simultaneity of PV generation and heating demand. In winter, the complete PV supply is almost entirely used to cover the electrical demand. In summer, there is high PV supply, but a negligible need for SH. The energy demand for DHW, however, is more or less constant over the year. Consequently, the load flexibility provided by DHW storages is also distributed more constantly over the year than the flexibility of SH storages, i.e. DHW storages provide a noteworthy load flexibility also in times of high PV supply. Hence, larger storages for DHW enable a higher self-consumption of the PV system and are, thus, more profitable than storages for SH, because of obtaining less energy from the external grid. The value of the SH storage is less in load shifting, but more in covering peak demands in winter, when the heat supply of the air-water heat pumps is also low due to low ambient temperatures of the air. The storage size of at least $17{,}7\mathrm{kWh_{th}}$ is caused by scenarios with very cold winters. Implicitly, the optimal storage size depends on the system component's capacities, i.e. the installed PV system and used number of heat pumps. For example, a larger PV system makes a larger storage more attractive, because more heat demand can be shifted to times when PV energy is supplied and the price for electricity is low. A heating system with more heat pumps could cover peak demands with smaller SH storages.

It could have been expected that the storage size for SH is more sensitive to uncertain meteorological parameters than for DHW. But there is a higher variation of the DHW storage in comparison to SH storage in both cases SLP (a) and SMILP (b), when the scenarios are optimized separately. The fact that the daily energy demand for DHW is more or less constant over the year and the demand for SH is mainly in winter indicates that the uncertainties on the supply side (i.e. PV generation) lead to this higher sensitivity in comparison to the uncertainties on the demand side (i.e. heat demand). However, in this case, it is not only the uncertain PV supply that influences the storage size. But it is the load shifting potential in general, which depends on the complex combination of time-depending PV supply and electrical and thermal energy demand. Furthermore, storage losses and ramp-up losses of the heat pumps influence the profitability of load shifting. If integer variables are involved, this influence is higher than with continuous heat pump power supply resulting in an increased sensitivity to uncertainty and a higher variation of the DHW storage in SMILP (Fig.5b) in comparison to SLP (Fig.5a).

The optimal storage sizes differ notably from the results when using expected values. However, if the investments were based on the results of the EV or even on the frequency peak of occurrence, there would be scenarios that are very expensive or, when the heat constraint is not relaxed, even infeasible. In contrast, the optimal solutions of the SLP and SMILP take all scenarios into account and result in a storage size that is not optimal for the specific scenario, but feasible for all scenarios and cost-minimal in expectation.

The variations of the costs are mainly driven by the PV supply and the thermal demand, both depending on uncertain, stochastic weather conditions: the higher the global solar radiation and temperatures of one year, the lower the minimal costs because of a higher PV supply and a lower thermal demand. The residual PV surplus of at least 44% up to 49% has to be fed into the external grid. Similarly, the autarky rate indicates which share of the total energy demand can be covered by the decentralized energy sources and how much energy is needed from an external supplier. In this residential quarter, an autarky rate of one third is achieved, meaning that two thirds need to be covered externally for the given energy system. Concerning the grid layout, it is important to know the maximal electrical load. Almost independent of the used heat pump technology, this maximal load is 57kW. The total electrical net consumption from the external grid approximately amounts to $60\ 000\text{MWh}_{\text{el}}$ and varies by $\pm 5\%$. If inverter heat pumps are used, the total electrical demand can be reduced by around 2%. The reason for that is the higher COP, because of less numbers of heat pump switches resulting in lower ramp-up losses. Such model results can, inter alia, be very useful to support contract designing with external energy suppliers or distribution grid operators.
When heat pumps can only run with a technically limited flexibility at half or full load, i.e. integer variables are used, then the minimal costs increase by about $600€$, because the heat pump is restricted by stepwise instead of continuous power supply. This inflexibility is compensated by larger storages which is the main reason for the higher minimal costs. The difference to the SLP solution delivers a lower bound amounting to a relative gap of less than 2%. The SLP can also be used to determine the ranges of the optimal storage sizes by maximizing and minimizing the sizes on the hyperplane with the same optimal objective value of the SMILP: At the fixed objective value of $31\,729€$, the SH storage can range between $17{,}7$-$87{,}1\text{kWh}_{\text{th}}$ and the DH storage between $23{,}8$-$160{,}6\text{kWh}_{\text{th}}$.

5. Discussion of the methodology

Commonly, when SP is applied for problems with uncertain data, the expected value of perfect information (EVPI) is indicated. It gives an economic value for obtaining perfect information about the future, so it is a proxy for the value of accurate forecasts. The EVPI is calculated as difference between minimal expected costs of the stochastic solution and minimal expected costs which are possible in the best case. ‘In the best case’ means that perfect information about future scenarios would be available and the storage size could still be adapted for each occurring scenario. Mathematically, these minimal costs can be determined by relaxing the non-anticipativity constraints. For the SLP and the SMILP, the difference is less than 1% meaning that the savings are marginal when the occurring scenario is known exactly and the storage size could be optimally adapted. Because each scenario is optimized separately by an exact branch & cut approach, that information can be used as an better relative gap for the SMILP.

The advantage of modeling the problem not deterministically, but as an SLP or SMILP, can be expressed by the value of stochastic solution (VSS): Thereby, the expected result of the EV solution (EEV) is subtracted from the optimal solution of the SP (Birge, 1981). The EEV is calculated by the optimization of the stochastic program using the EV solution, i.e. by minimizing the expected costs of the stochastic program using the storage sizes that are deterministically determined for the expected values of the uncertain input parameters. In both SLP and SMILP, the EV solution is not feasible for all scenarios without a relaxed heat constraint. Thus, the VSS is not quantifiable, but from a qualitative viewpoint, very valuable. If the decision was made on the basis of an optimization with expected values, there would be possible scenarios in the future with constraints that could not be satisfied. In the worst case, that could lead to a collapse of the real energy system. In this case study, constraints for the thermal demand could not be always satisfied meaning that there are time steps in the year where the room temperature is below the desired temperature of the inhabitants. Therefore, compensation terms, as proposed in chapter 4.b, are incorporated resulting in a VSS for the SLP of $56\,196€$ (177% more than the optimal solution of the SLP) and for the SMILP of $3\,725€$ (12% more than the optimal solution of the SMILP).

Critically reviewing our approach, SP is only applicable, when probability distributions of the uncertain parameters are known. The difficulty is to determine a distribution that adequately represents the actual distribution of the uncertain parameter. For the case study, a Markov process is used for simulating the uncertain parameters. The required transition probabilities are derived from historical data. On this basis, the computed solution is only optimal in expectation, when the future occurs as it is statistically derived from historical data base of over 50 years. Ahistorical occurrences or trends, e.g. the future climate development, could be taken into account by using model-derived forecasts or, if available, expert judgments. Besides determining the probability distribution, the number of scenarios, which represent the distribution sufficiently well, is difficult to choose.

For correct decision making, we should be aware that the optimal decision under uncertainties can also depend on risk preferences of the decision maker (Pflug & Misch, 2007). We wish to acknowledge that our results are purely based on economic considerations without accounting for subjective criteria.

For reasons of computational feasibility, each scenario is decomposed into 27 subproblems by fixing the heat storage sizes and the heat storage levels between the subproblems. The SH storage level between the subproblems is set to zero reasoned by the fact that this storage is not in use approximately in 5 of 12 months. For the DHW storage, a good estimation cannot be derived for the storage level. For this reason, the level is set to 50% of the storage size. These storage levels are not optimized to not increase the compositional effort needlessly. Thus, the solution is not exactly optimal. However, the error is negligible in this case study (error less than 0.1%). A SDP technique is not applied, because it disadvantageously results in a step-dependent optimization process and the possibility to independently optimize all 2700 subproblems in parallel would be dropped out.

Another option to deal with the problem size could be to reduce the temporal resolution of the problem. Our analysis shows that a reduction of the temporal resolution has a crucial impact on the optimal solution. For example, using time steps of one hour, the optimal storage sizes differ by more than 50% reasoned by a completely changed load shift potential within an hour instead of 15 minutes. It can be an option for handling large-scale stochastic programs, but this is very case-dependent. In general, it must be assumed that reduction of

temporal resolution leads to an insufficient solution that is too inaccurate for an application. On the opposite view, a temporal resolution of below than 15 minutes can even be required to achieve the needed accuracy. In principle, the developed approach and model can also be applied for smaller time steps. But besides the problem of an increased computational effort, there are nearly no consistent data available in a higher temporal resolution. In the case study with thermal storages as load shifting component, a temporal resolution of 15 minutes should be sufficient, because the profiles of thermal supply, demand and storing are smooth in comparison to electrical profiles, and there is no need to balance them at exactly the same time. When electrical storages are used for instance, then the sizes of the storages usually tend to be underestimated.
It should also be noted that continuous variables are used for the storage sizes for illustrative purpose. On the common market, only discrete sizes are available as economically reasonable investment. Then, integer variables have to be used that could even fasten the optimization process, because the hill-climbing approach searches only a finite number of combinations in comparison to infinite combinations of continuous storage sizes.

The advantage of the outer hill-climbing approach is that it needs few steps to come close to an optimum. In case of the SMILP, the disadvantage is that it can end in a local optimum when integers are involved. Even a more time-intensive evolutionary algorithm used by Till et al. (2007) as outer optimization can end in a local optimum. A global optimum can be guaranteed by either a complete enumeration or an exact algorithm like the mentioned branch-and-cut approach of Carøe et al. (1998, 1999) or Sherali et al. (2002, 2006, 2009) and the BFC methodology of Alonso-Ayuso, Escudero et.al (2005), Escudero et al (2007, 2010a, 2010b, 2012) and Pagès-Bernaus et al. (2015). But these approaches are prohibited by the problem size. For example, Pagès-Bernaus et al. (2015) apply their developed approach to two real instances with $447\,771$ variables (thereof $13\,338$ binary) and $56\,700$ variables (thereof $34\,479$ binary). An application to the case study of this paper with more than 100 Million variables would result in a non-performable computational effort that exceeds the current commonly available computing resources. At least, the solution of the SLMIP, relaxed either to a SLP or a program where the capacity can be adapted for each scenario separately, gives the gap to the minimal possible costs that indicates the applicability of the solution.

6. Conclusion and outlook

Within the paper, the optimization of the investment and operation planning process of a decentralized energy system is considered that is subject to different sources of uncertainties. Because of the complex impact of uncertain parameters on the solution, the investment decisions, such as the choice of an optimal storage capacity, derived from the stochastic solution can be very different from the solution based on expected values of the input data or the frequency peak of occurrence. Using two-stage stochastic programming leads to a solution that is optimal in expectation. This solution is much more reliable with respect to the parameter uncertainties than deterministic solutions which are not always feasible for all possible future scenarios. In general, thermal storages in such a quarter prove beneficial. The storage for domestic hot water is more profitable than for space heating due to the more constantly provided flexibility, particularly in events when heat demand can be shifted to times of PV peaks. A further key finding is that the beneficial effect of the storage for space heating is the fulfillment of all energy system restrictions, i.e. the covering of the heat demand, even in very cold winters. Therefore, the capacity for space heating is generally larger than the result of the deterministic optimization, e.g., with expected values. This added value can be expressed by the value of stochastic solution, which amounts to $56\,196$€ (177% more than the optimal solution), when inverter heat pumps are used, and to $3\,725$€ (12% more than the optimal solution), when heat pump can only run stepwise at idle, half or full load.

The presented module-based, parallel computing approach accounts for the uncertainties by generating and transforming consistent ensembles of data required for the stochastic optimization problem. Thereby, mutual dependencies of the uncertain parameters are taken into account and propagated consistently through the complete model chain. Although the problem ends up in a large-scale two-stage stochastic program, the used parallel optimization process and an outer hill-climbing optimization find an optimum in few steps reliably. It is also not anymore an issue of the problem size, but more of the available computer capacity. The approach is applied for a residential quarter with 70 households having a PV system and heat pumps in combination with heat storages.

The developed approach is used to support optimal decisions of investment in the long-term and their optimal operation in the short-term. In this context, an optimization with a high temporal resolution is required for an optimal operation of the investments in the short-term. As a consequence, the approach can also be applied for the real-time optimization of the operating energy management of the system. The investments are fixed and a rolling time horizon of the stochastic program is executed for a short-term period. Therefore, the scenario generation has to be adapted using current weather forecast services for generating required weather profiles considering their probabilistic forecast error.

Besides optimizing the storage size, other components, such as the PV capacity, can be optimized by the approach for further quarters. Additionally, technologies that are not yet integrated can be considered by adapting the optimization module. For instance, the economic value of an electrical storage and the optimal size could be determined. Furthermore, complex relationships and impacts could be analyzed as the electrical storage influences the decisions for the thermal storage. The conceptual framework can be also adapted to decentralized energy systems that have, for example, wind power or micro-combined heat and power systems or different types of energy demand. It gives the possibility to easily exchange the modules that generate ensembles of the uncertain parameters or that transfer these ensembles into energy supply and demand profiles.

We aim at further improvements in enhanced modules for energy demand profiles of the data transformation subsystem. In the current state, energy demand is derived by reference load profile approaches that cause further uncertainties. To reduce the introduced uncertainties, the load profiles could be extended by an additional error correction method. An alternative can be to supplement the standard load profiles with their statistical deviations. So the simulated weather profiles will be transformed into electrical and thermal demand profiles plus a simulated deviation based on measured data.

The conservative, robust consideration of satisfying all model constraint is relaxed by accepting heat supply below the demand with a high penalty term in the objective function. If the abidance of this restriction and the robustness of the solution have less priority, the approach of Good, Karangelos, Navarro-Espinosa, and Mancarella (2015) can be used that values the violation of heat demand constraints as ‘price of discomfort’.

Risk preferences can be incorporated by adding an additional term to the objective function: Instead of minimizing or maximizing an expected value, a combination of expectation and a measure of risk-preference is optimized.

The performance of the developed approach for SLP and SMILP can be improved by, e.g., a gradient decent instead of the hill climbing method and by using scenario reduction techniques. In case of SMILP, the approach could be extended by a subsequent stochastic search of the first-stage variables to ensure a globally optimal solution.

Appendices

Table 1: Nomenclature

Parameters	
ANF	annuity factor
$cost_i$	variable capacity costs of component i plus a fix amount
$COP_{\omega,u,t}$	COP of the heat pump in scenario ω of building group g for use u at time t
$d_{\omega,t}^{hp,max}$	maximal heating power of the heat pump at time t
$d^{he,max}$	maximal heating power of the heating element
$d_{\omega,t}^{ee}$	electricity demand for electrical usage in scenario ω of building group g at time t
$d_{\omega,g,u,t}$	thermal demand in scenario ω of building group g for use u at time t
$e_{\omega,t}^{pv,kwp}$	supplied electrical energy per kilowatt-peak of the PV system in scenario ω at time t
$e_{\omega,t}^{pv}$	supplied electrical energy from the PV system in scenario ω at time t
f	compensation factor for not-covered heat demand
l_u	loss factor of heat storage for use u
m	possible power modes of the heat pump
r_u	ramp-up loss factor of heat pump for use u
p^{grid}	price of electricity from grid
p^{fi}	price of feed-in compensation
η	efficiency of the heating element
Variables	
$c_{g,i}$	capacity of building group g of component i
$c_{g,i=PV}$	installed PV capacity of building group g
$c_{g,i=HP_{SH}}$	number of heat pumps of building group g for SH
$c_{g,i=HP_{DHW}}$	number of heat pumps of building group g for DHW
$c_{g,i=HE_{SH}}$	number of heating elements of building group g for SH storage
$c_{g,i=HE_{DHW}}$	number of heating elements of building group g for DHW storage
$c_{g,i=S_{SH}}$	maximal capacity of heat storage of building group g for SH
$c_{g,i=S_{DHW}}$	maximal capacity of heat storage of building group g for DHW
$d_{\omega,g,u,t}^{hp}$	used electricity of heat pump in scenario ω of building group g for use u at time t
$d_{\omega,g,u,t}^{he}$	used electricity of heating element in scenario ω of building group g for use u at time t
$e_{\omega,t}^{grid}$	used electricity from the grid in scenario ω at time t
$e_{\omega,t}^{fi}$	fed-in energy of the PV system in scenario ω at time t
$L_{\omega,g,u,t}$	losses of the heat storage in scenario ω of building group g for use u at time t
$pos_{\omega,g,u,t}$	pos. variable for positive shift of heat pump in scenario ω of building group g for use u at time t
$neg_{\omega,g,u,t}$	pos. variable for negative shift of heat pump in scenario ω of building group g for use u at time t
$q_{\omega,g,u,t}$	not-covered heat demand in scenario ω of building group g for use u at time t
$s_{\omega,g,u,t}$	stored heat in scenario ω of building group g for use u at time t
$s_{g,u}^{min}$	minimal heat storage level of building group g for use u
$z_{\omega,g,u,t}$	integer/continuous heating power level in scenario ω of building group g for use u at time t
Indices	
g	building group $1,..,G$ of the quarter with $G = 4$
i	component $i \in \{PV, HP_{SH}, HP_{DHW}, HE_{SH}, HE_{DHW}, S_{SH}, S_{DHW}\}$ of the energy system with $\|i\| = k_1 = 7$
u	use $u \in \{SH, DHW\}$ for space heating or domestic hot water with $\|u\| = 2$
t	time index $1,..,T$ indicating the time step of the year
ω	scenario index $1,..,N$

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