



Portfolio optimization in district heating: Merit order or mixed integer linear programming?

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ABSTRACT

Long-term portfolio optimization is commonly used to find the most cost-effective design and operation of a district heating system, subject to technical, financial, and environmental restrictions. Optimizing a district heating system is not trivial and demands high accuracy and high computational speed. However, existing methods addressing this problem offer one or the other but not both at the same time. The state-of-the-art method for portfolio optimization is mixed integer linear programming (MILP), which is extensively used in industry and academia but can be computing and resource-intensive for large portfolio models. This limitation has motivated the development of various options to reduce the computation time while maintaining the accuracy to a large extent. An alternative method to MILP is the merit order (MO) method, which has been used especially for power generation applications due to its simplicity and faster computation but somewhat reduced accuracy. The aim of this paper is to investigate the potential advantages and disadvantages of MO models compared to MILP models in the context of optimizing the portfolio of assets supplying a district heating network. As a study case, we analyze a large portion of the district heating network in Berlin. Four MO model variants with different levels of complexity are proposed and compared to a reference MILP model. Results suggest that MO models variants including heat storage and describing CHP plants with significant detail have the potential to reduce calculation time by nearly three orders of magnitude compared to the reference MILP model, without significantly sacrificing accuracy. In fact, differences in heat generation and net present value (NPV) between the most accurate MO model and the reference MILP model account for $\pm 4\%$ and -6% , respectively. Moreover, results show that combining MO and MILP models is advantageous and offers high computational speed and at the same time high accuracy, especially when a large number of runs might be necessary. MO models could thus be used prior to MILP models to perform a pre-evaluation, an exploration of sensitivities, or for downsizing the initial optimization problem. Combining MO and MILP models could result in faster and more robust decision-making, which could otherwise not be attained with any of the two options individually.

1. Introduction

Germany aims to become greenhouse gas neutral by 2045 [1]. Similarly, the state of Berlin has set a goal of phasing out the use of coal by 2030 at the latest, and of becoming climate-neutral by 2050 at the latest [2]. One of the priorities to achieve carbon neutrality is the decarbonization of the heat supply, which currently contributes to 50% of the final energy demand (66 TWh per year) and is 90% based on fossil fuels [3]. Designing a sustainable, affordable and climate-neutral heat supply for Berlin is therefore essential. However, this is not a trivial task. From a planning perspective, Berlin lacks low-carbon heat sources for

heat generation, such as geothermal, industrial waste heat or biomass, unlike other cities in Europe. From a computational perspective, the complex network and portfolio, as well as the large number of uncertainties, require simulation tools that are fast and accurate. This challenge has already been addressed in various studies. For example, Berlin's Senate Administration for the Environment, Transport and Climate Protection (SenUVK) together with the district heating operator (Vattenfall) have identified climate-friendly transformation paths to replace existing coal-fired power units for district heating in Berlin by 2030 [4]. Fraunhofer IEE has also identified potential sources and technologies for achieving a climate neutral heat supply in Berlin by 2035 [5]. These studies suggest that to achieve carbon neutrality it is

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Nomenclature		NPV	Net present value
		N	Net cash flow
		O&M	Operation and maintenance
		p	Price
		P	Production
		P2H	Power-to-heat, i.e., electric boiler
		Q	Heat generation
		r	Electricity revenues
		ROA	Real-options analysis
		sc	Specific variable operational and maintenance cost
		SA	Supply area
		SenUVK	Berlin's Senate Administration for the Environment, Transport and Climate Protection
		TPI	Third party integration
		VC	Variable costs
		η	Efficiency
		λ	Power-to-heat ratio
C	Costs		
CHP	Combined heat and power		
COP	Coefficient of performance		
E	Power generation		
F	Energy input		
FC	Fixed costs		
HOB	Heat-only boiler		
HPC	High-performance computing		
k	Specific CO ₂ emission factor associated to the energy input		
LP	Linear programming		
MC	Marginal costs		
MILNP	Mixed integer non-linear programming		
MILP	Mixed integer linear programming		
MO	Merit order		
MVP	Mean-variance portfolio analysis		
NGCC	Natural gas combined cycle		

necessary to modernize the existing heat supply portfolio, which requires large investments in technologies with lifetimes spanning several decades. Identifying an optimal portfolio requires a dedicated analysis of investments, risks and cost-effectiveness of different variants, a process which is commonly carried out using a framework for long-term portfolio optimization [6].

Portfolio optimization is a methodology to address the challenge of finding the most effective combination of individual producing units to supply the demand of a product or service while minimizing or maximizing other criteria (e.g., emissions, investments, operational costs, etc.) and satisfying certain restrictions (e.g., supply the demand). Portfolio optimization is also commonly used as an effective strategy for risk hedging, i.e., combining multiple individual units leads to a reduction in the probability of supply disruptions [7]. In the context of energy generation, portfolio optimization is used to find the optimal investment and/or operation of a portfolio of multiple individual assets, aimed at supplying the energy demand of a user within concrete boundary conditions and subject to various constraints [8,9]. Typical criteria for portfolio optimization include minimizing investment or operational costs, minimizing risks (understood as the variability in costs, availability or other measures), or minimizing associated emissions. Often the problem involves multiple conflicting criteria to be optimized simultaneously, which requires a tradeoff curve or Pareto solution [8].

From a mathematical point of view, the modeling approaches for portfolio optimization can be stochastic (i.e., when the variables of the system appear to vary in a random manner) or deterministic (i.e., when no randomness is involved) [7,8,10]. Methods for portfolio optimization following a stochastic approach include the mean-variance portfolio analysis (MVP), the real-options analysis (ROA), Monte Carlo simulation, multi-criteria decision analysis or combinations thereof [7,10]. These methods aim at maximizing profit associated with power generation while simultaneously minimizing the associated risk or uncertainty. Methods for portfolio optimization using a deterministic method include linear programming (LP), merit order (MO), mixed integer linear programming (MILP) and mixed integer non-linear programming [11]. MILP and MO are the most used methods, and both aim at determining the optimal dispatch of the generation units and minimize the overall operational costs, subject to various constraints [11]. The MILP approach includes integer decision variables and considers a rich technological detail, including part-load characteristics, start and turn-down strategies, etc. [11]. The MO approach follows the merit order, which is the ranking of the plants according to their ascending marginal costs of production. The MILP approach offers a more realistic representation of reality compared to the MO approach, and it is significantly more time-

and computational-intensive. In the context of district heating or combined heat and power (CHP) supply, deterministic methods are the most commonly methods for portfolio optimization, even though there are some examples using stochastic methods [12,13].

As the complexity of energy systems grows because of integrating more renewable energy sources and storage technologies, so does the computational challenge to achieve accurate results in a reasonable amount of time. To address this issue, an approach used in the literature has been to investigate to what extent simplifying a model or employing a simpler method can affect the results [11]. For example, in the power generation context, Cebulla and Fichter [11] described various studies that compared MO against MILP. These studies have shown that the importance of technological detail in power plant modeling increases with greater demand for flexibility, thus neglecting technical constraints can lead to sub-optimal portfolios.

However, to the best of our knowledge, comparisons between MO and MILP in the existing literature have so far been limited to power generation. Thus, the novelty of this paper is to extend the comparison of these two methods to district heating and CHP supply. MILP and MO have been individually applied to these sectors in the past, but their capabilities have so far not been compared for a given study case. This paper aims at filling this gap. We compare a state-of-the-art MILP model against various proposed MO models with different degrees of complexity for optimizing the portfolio of assets serving a portion of the district heating network in Berlin, the largest in Germany. The proposed MO models also offer improved features compared to similar models in the prior studies, for example the inclusion of heat storage and a detailed depiction of CHP plants, e.g., a heat vs. power generation map at full-and part-load.

This comparison is not intended to be mathematically exhaustive, as many of the details considered in MILP models are not easily reproducible or translated into MO models. Instead, the comparison intends to be exploratory and to identify advantages and disadvantages. We focus on optimizing the long-term operation of a given portfolio and therefore the optimization of its design or investment is not considered.

The approach consists of three steps. Firstly, we analyze the characteristics, advantages and challenges of each method. Secondly, we build a reference MILP model and various proposed MO model variants and apply them to analyze a portion of the district heating grid in Berlin as a study case. For the MO model, we evaluate different variants that describe the flexibility of the system with varying degrees of accuracy. Thirdly, we compare the differences in heat and power generation as well as the associated heat generation costs, NPV and computational time for the different methods. Moreover, we investigate the

combination of MO and MILP models to evaluate whether there is a potential improvement in computational speed and accuracy compared to any of the two options individually.

The presented methods and results could be relevant for system operators and policy makers in the district heating and heating sectors seeking improved decision-making for planning of generation and grid capacity, decarbonization of the supply, and risk mitigation.

This paper is structured as follows: Section 2 presents a description and comparison of MILP and MO models in the context of district heating and CHP; Section 3 describes the methodology followed in this paper; Section 4 sets out results; Section 5 presents a discussion; Section 6 draws conclusions.

2. Modeling approaches to portfolio optimization

2.1. Mixed integer linear programming (MILP)

MILP is the most widely used method for dispatch optimization in energy supply applications, employed in hundreds of studies in the literature. The main objective is to supply the demand while minimizing the overall costs or maximizing the profit of the system. The optimization problem can be further categorized into three levels [14,15]: a) optimization of the system configuration, b) optimization of the components' design and characteristics and c) optimization of the operation of the system.

A typical MILP approach for optimizing the operation of an energy system is described below [16]:

Objective function:

$$\text{Max/Min} \sum_{j=1}^n c_j x_j \quad \text{Eq. 1}$$

Subject to the following constraints:

$$\sum_{j=1}^n a_{ij} x_j \leq b_i \quad \text{Eq. 2}$$

$$\sum_{j=1}^n d_{ij} x_j = e_i \quad \text{Eq. 3}$$

Nonnegativity condition:

$$x_j \geq 0 \text{ for all } j = 1, \dots, n \quad \text{Eq. 4}$$

where x_1, \dots, x_n are the optimization variable s, c_j are the coefficients of the variables ($j = 1, \dots, n$), and a_{ij}, d_{ij} are constant coefficients of the constraints ($i = 1, \dots, m$). The optimization variables can be real numbers ($x_j \in \mathbb{R}$), integers ($x_j \in \mathbb{Z}$) or binary numbers ($x_j \in \{0, 1\}$).

The optimization problem aiming at minimizing costs or maximizing profits is further complicated in polygeneration systems, where multiple demands must be simultaneously met while satisfying additional constraints. In the context of district heating and CHP, the system must satisfy the heating demand and can also generate electricity. Optimization of district heating supply using MILP is a well-studied problem in literature, e.g., Refs. [17–24]. For example, Gonzalez-Salazar et al. have used MILP to find optimal combinations of supply technologies to serve six demand cases, three commercial applications and three residential applications [17,18]. Lezko et al. have used MILP to optimize a district heating system with capacity- and temperature-limited sources, addressing thermal energy storage in the building inertia [19]. Pantaleo et al. have optimized the spatial and temporal allocation of biomass supply, storage, processing, transport and heat and power generation to supply a district heating network [21]. Capuder and Mancarella have proposed an optimization framework based on MILP, to compare distributed multi-generation technologies for district heating supply [22]. Ameri and Besharati have used MILP to optimize the capacity and operation of seven combined cooling, heating and power systems in

Tehran [23]. Ghilardi et al. used MILP to optimize the heat supply in a group of buildings in Parma featuring the exploitation of the heat capacity of building to increase flexibility [24]. Kouhia et al. has investigated the influence of different design functions using MILP on the configuration of district heating systems [25]. In addition, various studies have focused on evaluating the heat storage influence on the performance of district heating systems [26–29]. Multicriteria optimization of district heating systems has been addressed by Rieder et al. [30] and Buoro et al. [31]. Finally, the optimal design and operation of district heating or CHP system has been investigated in various studies [32–36].

The advantage of MILP is twofold. Firstly, it guarantees finding a global optimal solution, and secondly it can use a wide variety of commercial and open-source solvers [14]. However, MILP involves practical limitations such as the large number of variables required to include decisions about the configuration and design of the system and the impossibility to address non-linear effects. This increases the computational effort and makes the results less easy to process and interpret.

To solve the issue of a large number of variables, various approaches have been proposed, including a) dimensionality reduction and b) linearization of system variables. Dimensionality reduction aims at decreasing the size of input data by clustering data using k-means, k-medoids or similar algorithms [20,37]. Linearization of system variables relates to the conversion of binary variables into continuous variables for a first approximation, which is then used as a proxy value for a real run [14]. In this approach the MILP optimization problem is converted into a linear programming problem. Linearization is also commonly used to approximate various non-linear functions such as the efficiency of the components in part-load, the performance of units as a function of ambient temperature, thermal losses, etc. [38–40].

2.2. The merit order (MO) method

The merit order is a method to rank supply units according to their ascending marginal costs. In economic theory, the marginal cost refers to the cost added by producing one additional unit of a product [41]. The marginal cost MC is defined as the first derivative of a cost function C with respect to production quantity P :

$$MC(P) = \frac{dC}{dP} = \frac{d(FC + VC)}{dP} = \frac{d(VC)}{dP} \quad \text{Eq. 5}$$

The cost function consists of fixed costs FC and variable costs VC . As the fixed costs do not change when the production quantity varies, the marginal cost is the first derivative of the variable costs with respect to the production quantity. The MO method has been relevant for long-term portfolio planning because of its robustness and simplicity. In fact, the MO method has been the predominant pricing method in most of the existing electricity markets [42–44] and the fundamental concept behind various renowned energy modeling frameworks for portfolio optimization, including MARKAL/TIMES [45], and the World Energy Model (WEM) [46].

In the context of CHP and district heating, various studies have used the concepts of marginal costs and merit order for dispatch optimization. Josefsson et al. have created the 'Martes Model', which is a merit order dispatch model used for analyzing the profitability of investments, budgeting, emissions, and marginal costs [47]; this model has afterwards been used to estimate the marginal cost of a district heating system in Sweden [48] and the Netherlands [49]. Moser et al. point out that the so-called Heat Merit Order is not a widespread concept for many researchers and therefore apply it for estimating the value of industrial waste heat used in district heating networks [50]. Similarly, Hofmeister et al. use marginal costs and MO order combined with a model predictive control as dispatch strategy for optimizing a heating network of a midsize town in Germany [51]. Dominkovic et al. have used these methods to evaluate reference system costs for study cases in Denmark and Finland, as well as potential improvement through dynamic pricing

[52]. Moreover, Delmastro et al. use a merit order approach to evaluate a combination of district heating and building renovation options in Italy and Sweden [53].

The marginal costs of heat generation in a district heating network can be evaluated as follows. There are units generating heat only (e.g., heat-only boilers, electric boilers) and units generating heat and power (e.g., gas and steam turbines). The marginal cost of heat generation by technology can be defined as:

$$MC(Q) = \frac{dC}{dQ} = \frac{d(VC)}{dQ} \quad \text{Eq. 6}$$

$$MC(Q) = \frac{d(C_{Input} + C_{CO2} + C_{O\&M} - r_{Electricity})}{dQ} = \frac{d(C_{Input})}{dQ} + \frac{d(C_{CO2})}{dQ} + \frac{d(C_{O\&M})}{dQ} - \frac{d(r_{electricity})}{dQ} \quad \text{Eq. 7}$$

where Q is the heat generation, C_{Input} are the costs for energy inputs, C_{CO2} are the costs associated to CO_2 emissions, $C_{O\&M}$ are the variable operational and maintenance costs and $r_{Electricity}$ are the revenues received by generating and selling electricity. Eq. (7) can be reformulated as:

$$MC(Q) = \frac{d(p_{Input} \bullet F_{Input})}{dQ} + \frac{d(p_{CO2} \bullet k_{Input} \bullet F_{Input})}{dQ} + \frac{d(C_{O\&M})}{dQ} - \frac{d(p_{electricity} \bullet E)}{dQ} \quad \text{Eq. 8}$$

where F_{Input} is the energy input (MWh) such as fuels, electricity, etc. And p_{Input} is the associated price for energy inputs (€/MWh)¹; p_{CO2} is the carbon price (€/ton CO_2); k_{Input} is the specific CO_2 emission factor (ton CO_2 /MWh) associated to the energy input; $p_{electricity}$ is the price of electricity and E is the power generation. Eq. (8) can also be expressed in terms of efficiencies:

$$MC(Q) = \frac{p_{Input}}{\eta_{th}} + \frac{p_{CO2} \bullet k_{Input}}{\eta_{th}} + sc_{O\&M} - p_{electricity} \bullet \lambda \quad \text{Eq. 9}$$

where η_{th} is the thermal efficiency of the technology (dQ/dF_{Input}); λ is the power-to-heat ratio for CHP plants (dE/dQ), which can be also expressed as the ratio of electrical efficiency (η_e) to thermal efficiency (η_{th}); and $sc_{O\&M}$ is the specific variable operational and maintenance (O&M) costs (€/MWh). For technologies generating heat only, such as heat only boilers, the revenues from generating and selling electricity are zero (λ is zero). For technologies converting electricity into heat, such as heat pumps, the energy input is electricity, and the thermal efficiency is the coefficient of performance (COP).

Eq. (9) shows that the marginal cost for heat generation for any type of technology depends on economic parameters such as prices (price of energy input and CO_2) and specific costs, as well as on technical parameters such as the thermal efficiency and the specific emission factor associated to the energy inputs. Electricity prices also play an important role for technologies converting power into heat or vice versa. For example, for CHP technologies, the marginal costs also depend on the electricity revenues, which are in turn a function of the electricity prices and their ability to generate power (i.e., the power-to-heat ratio). Electricity prices also strongly influence the marginal costs of technologies converting electricity into heat, such as electric boilers and heat pumps, especially compression heat pumps.

For a thorough analysis of the marginal costs of heat generation, it is useful to illustrate their relationship to the electricity prices. Fig. 1 (top) shows exemplary marginal costs of heat generation for various

technologies, viz. A gas boiler, a heat pump, a gas turbine and a natural gas combined cycle (NGCC), as a function of electricity prices.² The figure shows that while the marginal cost is independent of the electricity price for the gas boiler, it is positively correlated to the electricity price for the heat pump and negatively correlated for the gas turbine and NGCC. For these two latter cases, the higher the power-to-heat ratio, the steeper the negative slope of the curve. A merit order, or dispatch order, is estimated by ranking the different technologies according to their ascending marginal costs, see Fig. 1 (bottom). In this example, the most economical technology up to an electricity price of 60 €/MWh is the heat pump and from this point onwards it is the combined cycle.

In a district heating system with a portfolio consisting of multiple generation assets, the marginal cost of the system equals the marginal cost of the asset with the largest marginal costs required to supply the demand [54]. This can be seen in an exemplary merit order curve in Fig. 2, where the marginal cost of the system in order to meet the demand is the marginal cost of the unit “1”.

2.3. Comparative overview

The complexity of today's energy systems is continuously growing among others because of stringent climate targets, increased flexibility to backup growing renewables [55], higher temporal and spatial resolution [56], as well as large uncertainties associated to fuels price and availability. To address this growing complexity, approaches for portfolio optimization no longer need to find the optimal solution for a single given set of assumptions, but instead to identify the solution that performs the best under a large number of assumption sets (i.e., scenarios), see Fig. 3. By evaluating a single set of assumptions, it is possible to quantify the model's accuracy but not its precision, i.e., the model response to variability or uncertainty.

MILP offers multiple advantages. For example, when optimizing CHP and district heating systems, MILP considers detailed technical and economic characteristics of generation technologies, sub-grids and their interconnections, as well as other factors such as energy storage, impacts of weather on technology performance, supply and return temperatures

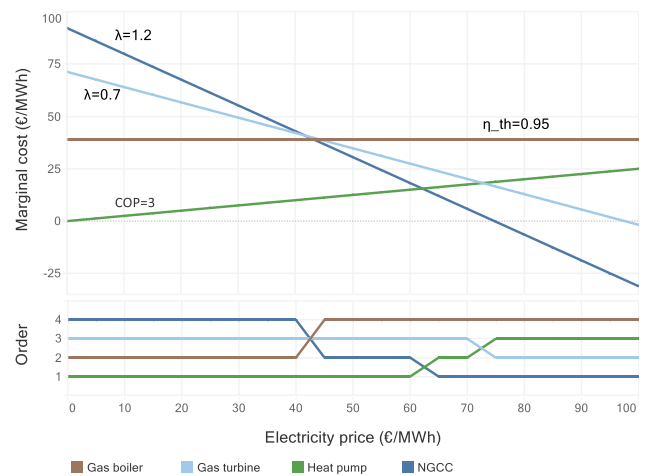


Fig. 1. Marginal costs of heat generation for various technologies as a function of electricity price (top), and the associated merit order (bottom).

¹ This price should be as close to the market price as possible, thus it should include taxes, fees, levies, etc.

² Assumptions include a 95% thermal efficiency for the gas boiler; a COP of 3 for the heat pump; a thermal efficiency of 52% and a power-to-heat ratio of 0.7 for the gas turbine, a thermal efficiency of 40% and a power-to-heat ratio of 1.2 for the NGCC; additionally, a natural gas price of 25 €/MWh and a CO_2 price of 60 €/ton.

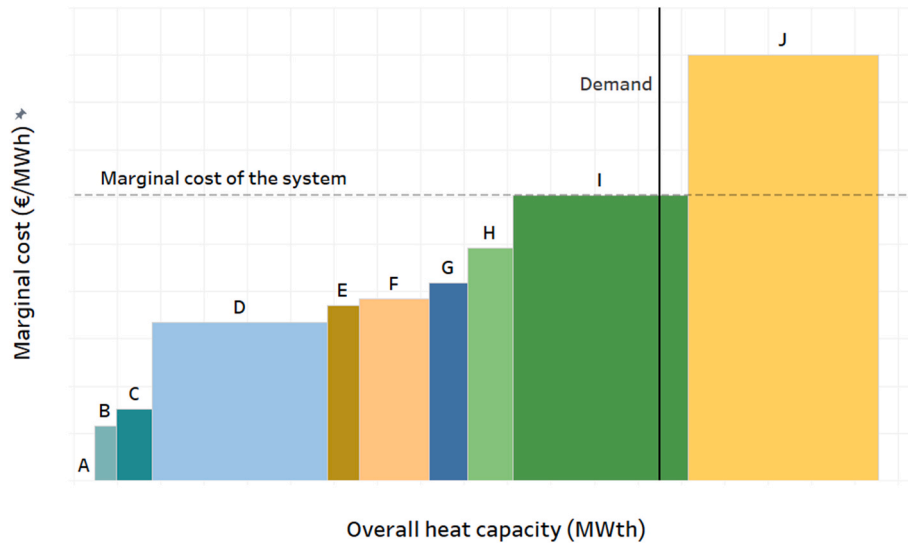


Fig. 2. Example of a merit order ranking.

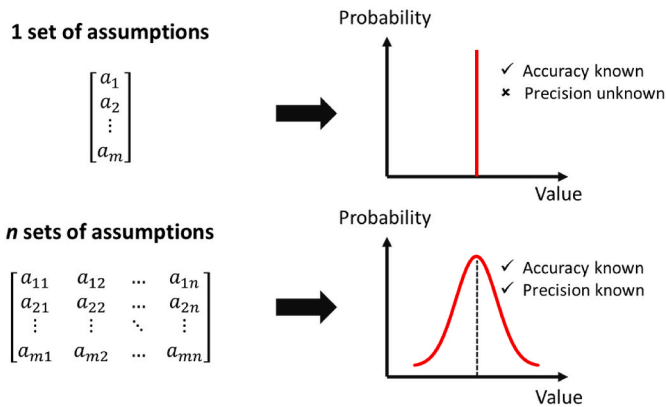


Fig. 3. Comparison of models considering different sets of assumptions.

of the grid, etc. Moreover, MILP guarantees finding a global optimal solution and can use a wide variety of commercial and open-source solvers. However, MILP suffers of the curse of dimensionality as well as the impossibility to address non-linear effects. Consequently, MILP is computationally- and time-intensive and often requires linearization methods to address non-linear effects. MILP's high accuracy sacrifices calculation speed, which limits its ability to timely evaluate multiple sets of assumptions. A possible solution is to parallelize computations using high-performance computing (HPC), but with additional costs and effort [56].

The merit order (MO) method is the predominant pricing method in electricity markets and is the concept behind various energy modeling frameworks. It is based on the concept of ranking supply units according to their ascending marginal costs, which are a function of their technical characteristics and prices. While in its standard form the MO method captures various technical and economic insights, some other details are not considered for the sake of simplicity. Topics often not addressed by the MO method include operational flexibility of power plants, off-design performance of energy technologies, supply and return temperatures in district heating systems, and energy imports or exports to other sub-grids. This inherent simplicity translates into a reduced computational effort than MILP, which becomes especially critical when running a large number of scenarios. The key question is to what extent this reduced computational effort implies a reduction in accuracy. This is the main question we aim at addressing in this paper.

3. Method

3.1. Approach

The approach followed in this study consists of three steps, see Fig. 4. In the first step, a study case to be evaluated with MILP and MO models is defined. Boundary conditions as well as technical and economic assumptions are also defined. In a second step, MILP and MO models are created to simulate the study case. Then, various MO model variants that address differently the operational flexibility of CHP plants and heat storage are evaluated. Flexibility in this context means the ability of CHP plants to independently generate heat and power, which in other studies is known as 'product flexibility' [57]. Finally, in the third step, results of the different models are compared and analyzed. Key measures for comparison include heat and power generation, the associated heat costs and the sum of the discounted values (i.e., NPV), as well as the computation time. These three steps are described in more detail in the flow chart below.

3.3. Study case

3.3.1. Challenge

Berlin has set the goal to become carbon-neutral by 2050, which requires a full decarbonization of the district heating supply. Hence, it is urgent to find an optimal portfolio of technologies that ensures climate-neutrality and profitability. However, this is a challenging task from a computational perspective. On the one hand, the complexity of the system is high and likely to increase. The district heating system in Berlin is the largest in Germany and the third largest in the EU-27, accounting for a total grid length of 2000 km and a heat demand of 10.7 TWh per year [4]. Additionally, the energy market conditions are highly volatile, in particular prices (fuels, electricity and carbon) and resource availabilities. On the other hand, existing (commercially available) tools used for portfolio optimization are time- and resource-intensive. While these tools perform dispatch optimization, they typically do not include investment optimization. Thus, to find an optimal portfolio and address the associated uncertainties and risks, a common practice is to run multiple scenarios. However, the number of scenarios to consider is limited by the lengthy computation time required. It is key to find methods for portfolio optimization that are as fast and accurate as possible.

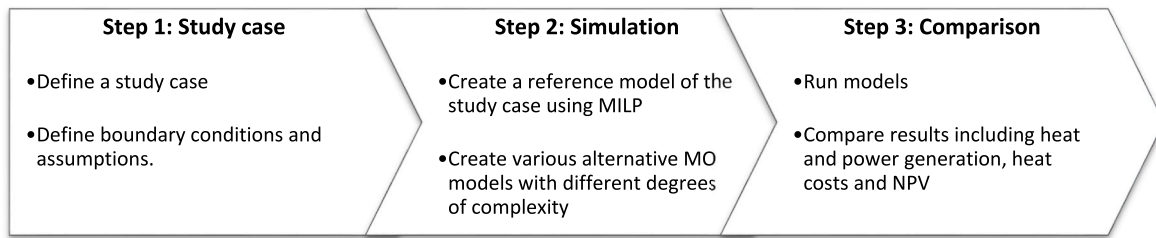


Fig. 4. Approach for comparing MILP and MO models.

3.3.2. Characteristics of the system

The defined study case is a so-called supply area within the district heating network in Berlin. The district heating network is divided into two main supply areas that are interconnected through a pipeline, namely Supply Area 1 (SA1) and Supply Area 2 (SA2). We concentrate on SA1, which extends over the western part of the city and demands nearly 4.7 TWh per year of district heat. A scheme of SA1 is shown in Fig. 5, where blue circles represent sub-grids (i.e., large groups of users), yellow boxes represent generation sites and red circles represent feed-in hubs, i.e., points where generation sites feed heat into the network. Red lines depict pipeline interconnections between generation sites, while black lines depict feeding lines. SA1 consists of three large groups of users or sub-grids: a) sub-grid North, b) sub-grid South and c) sub-grid Moabit. Six generation sites supply heat to those sub-grids, including Reuter, Reuter West, Moabit, Charlottenburg, Wilmersdorf, and Lichterfelde. Grid constraints exist due to limited pipeline capacity between generation sites. SA1 is a three-pipe-system: i) a heating pipeline with a variable supply temperature ranging from 80 to 110 °C depending on ambient temperature, which is operated during the heating season (see Fig. 6); ii) a smaller second pipeline with a constant supply temperature of 110 °C, which is operated throughout the year; and iii) a return flow with temperatures ranging between 50 and 60 °C.

Since our goal is to compare the performance of MILP and MO models in the long run, a time horizon starting in year 2030 and finishing in year 2050 is assumed. The assumed thermal and electrical capacities grouped by technology are shown in Table 1. In addition to these capacities, the assumed system includes two heat storage facilities (hot water tank storage at atmospheric pressure), one in Reuter West with a capacity of 2760 MWh and another one in Lichterfelde with a capacity of 1100 MWh. The assumed heat demand including the net heat transfer from SA1 to SA2 is shown in Fig. 7, with a peak demand around 2000 MW. In addition, assumed average non-discounted prices of natural gas, electricity and CO₂ are shown in Fig. 8.

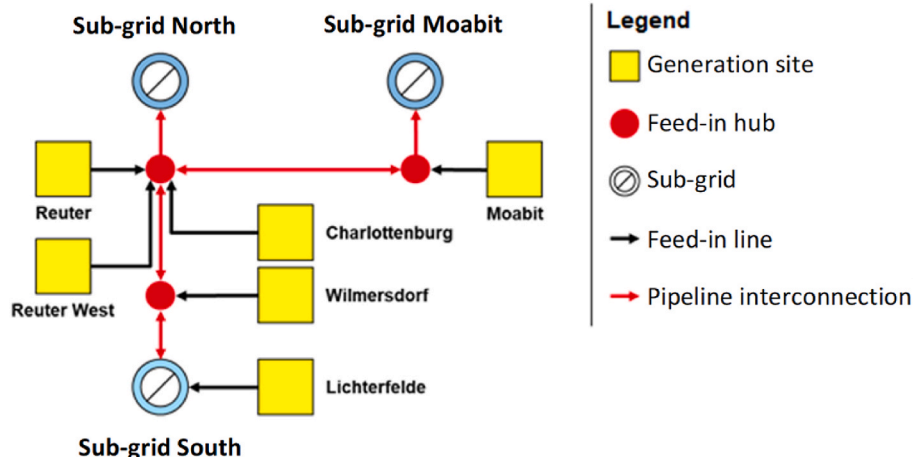


Fig. 5. Representation of Supply Area 1 (SA1) of the district heating network in Berlin.

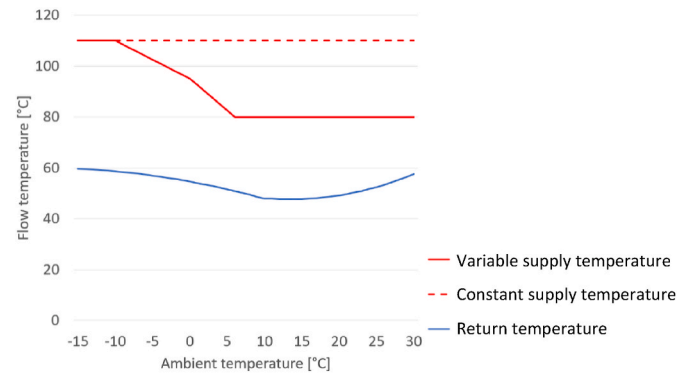


Fig. 6. Dependence of the supply and return temperatures on the ambient temperature.

Table 1

Assumed total thermal and electrical capacities (MW) by technology type.

Technology	Electrical	Thermal
Bio HOB		90.0
Gas CHP	714.3	793.0
Gas HOB		660.0
Geothermal		96.0
P2H		720.0
TPI	18.0	208.4

3.4. MILP model

A MILP model representing the study case is created using the commercial software BoFit [58], which is a well-established tool for portfolio optimization of district heating systems. The model offers a high level of detail and comprises all supply areas in Berlin including

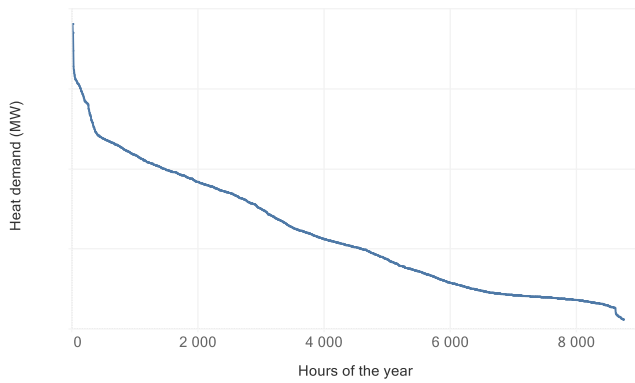


Fig. 7. Typical heat demand in Supply Area 1 (aggregation of the three sub-grids and heat transfer to Supply Area 2). The peak demand is close to 2000 MW_{th}.

generation islands not connected to SA1 or SA2. The model has been developed over multiple years and is considered the reference for our analysis. While the model accuracy may vary for different MILP implementations, we use the term MILP throughout the paper to describe this reference implementation of a MILP-based energy system model for portfolio optimization.

The model considers a temporal resolution of 4 h and includes various important features. Firstly, it allows a detailed depiction of flexibility of CHP plants, i.e., their ability to independently generate heat and power at full- and part-load. This information is entered as a heat vs. power diagram or ‘map’, which is dependent on ambient temperature. Secondly, it considers all capacity restrictions of the grid caused by limitations in pipeline interconnections between generation sites. Thirdly, it considers the supply and return temperatures of the district heating network, which are also dependent on the ambient temperature. Fourthly, it includes heat storage technologies, which enable daily or seasonal storage.

The objective function in this case is to minimize the overall operational costs of the total system:

$$\text{Min} \sum_{j=1}^n c_j x_j \quad \text{Eq. 10}$$

where x_1, \dots, x_n are the optimization variables and c_j are the coefficients

of the variables ($j = 1, \dots, n$). It is important to mention that this objective function does not include the capital costs for the different technologies, only operational costs. The objective function is subject to multiple constraints and the nonnegativity condition. The model consists of roughly 800 thousand continuous variables, 150 thousand integer variables and 1700 constraints. The model has a total time horizon of 20 years and performs the optimization on a quarterly basis, which means the solver gets called 80 times sequentially. The commercial solver Gurobi is used for solving the mathematical problem described above [59]. For running the MILP model, a computing server with 128 GB in RAM and 24 processors is used.

3.5. MO model

3.5.1. MO model variants

We develop four MO models with different levels of complexity, in order to identify which features have the most influence on the accuracy of the results and the calculation time compared to the MILP reference case. The MO models share some features with the MILP model but differ in others. An overview of the characteristics of the different models is shown in Table 2.

The MO models consider exactly the same technology portfolio and capacity restrictions of the grid as the MILP. However, the MO and MILP models differ in the form of addressing the heat transfer between sub-grids and the variation in supply and return temperatures of the network. While the MILP model allows to optimize the costs of the system and allows to transfer heat between sub-grids (sub-grid North, sub-grid Moabit and sub-grid South), these MO models optimize sub-grids individually and do not consider heat transfer between them. While the MILP model allows consideration of supply and return temperatures that vary throughout the year, these MO models assume them to be constant. Simulating the supply and return temperatures of the heating network demands a fully hydraulic representation of the network as well as additional thermodynamic assumptions to ensure that all assets achieve the supply temperatures. This is an added complexity of the MILP model that is contrary to the simplicity of the MO models, and hence has been considered out of scope. As a result, considered MO models are less descriptive and more conservative than the reference MILP model. For example, in MO models, heat pumps should always supply the highest supply temperature. To ensure this, a constant COP is used, which is not the technically highest for the heat pump. These are acknowledged simplifications of the MO models that still allow a feasible solution to be found.

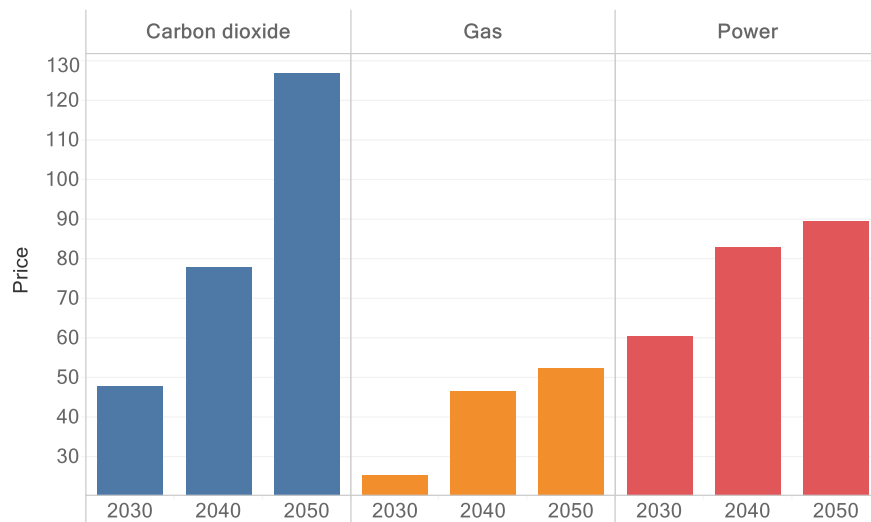


Fig. 8. Assumed average non-discounted price of natural gas (€/MWh), power (€/MWh) and CO₂ (€/ton CO₂).

Table 2

Overview of the features of the different models.

Model	Variant	Capacity restrictions	Heat transfer between sub-grids	Variation in supply and return temperatures of the network	CHP Flexibility	Heat storage
MILP	Reference	✓	✓	✓	✓	✓
MO	Variant 1	✓	×	×	✓	✓
MO	Variant 2	✓	×	×	✓	×
MO	Variant 3	✓	×	×	×	✓
MO	Variant 4	✓	×	×	×	×

Moreover, there are two features included in the MILP model that are considered differently in each of the investigated MO models. These two key features are: i) inclusion of multiple possible operating points for CHP plants and ii) inclusion of heat storage. Four combinations are thus defined, which reflect the ability of the models to consider either the flexibility of CHP plants, or the heat storage, or both, or none (see Table 2). The MO models are built upon the mathematical formulation described in Eq. (8) and Eq. (9). The MO models are built in Python, using various libraries for vectorization (NumPy), and data processing and analysis (pandas, seaborn). An important difference between the reference MILP and the MO models, is that the former is performing the optimization every quarter (80 times for a time horizon of 20 years) while the latter is performing the MO optimization every 4 h (43,800 times for a time horizon of 20 years). From an algorithmic point of view, the MO models investigated here are heuristic and apply a brute-force search, meaning that they systematically enumerate all possible solutions and then check the solution with the lowest associated costs every 4 h. For running the MO models, a personal computer with 32 GB of RAM and 4 processors is used.

3.5.2. MO model with CHP flexibility and heat storage (Variant 1)

The MO model including CHP flexibility and heat storage features is the most detailed variant. To find the cheapest solution, this variant uses a two-step strategy, as shown in Fig. 9. Firstly, the model finds the operating point with the lowest associated marginal cost for energy conversion plants offering multiple operational possibilities like CHP plants. Then, the model finds the merit order curve at a sub-grid level and at every time step. For this purpose, generation sites are grouped by the sub-grid they are feeding.

This strategy aims at mimicking the optimization approach of the MILP model, although with a substantial lower level of detail on various aspects. Firstly, the complexity of heat vs. power map is significantly reduced compared to the MILP model. This is accomplished by reducing the number of possible operational possibilities (i.e., the number of operating points in the map) and by ignoring the influence of ambient temperature on the performance of the plants. This is illustrated in Fig. 10, which compares the heat vs. power map for an exemplary CHP plant in the MILP and MO models.

To be on the conservative side, we assume that the plants always operate at an ambient temperature of -14°C , which knowingly leads to an overestimation of power generation and an underestimation of heat generation when the actual ambient temperature is higher than -14°C (most of the time). Additionally, this model does not consider temperature variations in the supply and return temperatures of the district heating network, in contrast to the MILP model. Instead, it considers fixed supply (110°C) and return temperatures (60°C) throughout the year. Secondly, as mentioned above, the MO model does not consider

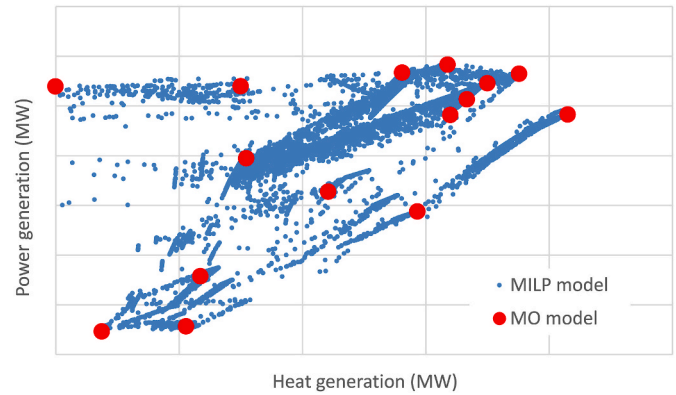


Fig. 10. Heat vs. power generation map for an exemplary CHP plant in the MILP and MO models.

heat transfer between sub-grids. In other words, it finds the merit order curve to supply the demand for each sub-grid but does not consider heat transfer between sub-grids. Thirdly, the MO model follows a simplified approach for simulating the heat storage. In this approach heat is stored only if the marginal cost of the system in a time step t is lower than during any of the subsequent 12 h. If the opposite occurs, heat is discharged. Heat can be accumulated and is kept below the maximal capacity of the heat storage unit. For simplicity, the efficiency of the heat storage is assumed to be 99% and to remain constant regardless of how the unit is operated.

3.5.3. MO models without CHP flexibility

MO models without CHP flexibility are a simplification of the variant described above. In this case, CHP plants are simply described with a single operating line in the heat vs. power generation map. This line starts in zero and goes up to the full-load point corresponding to an ambient temperature of -14°C . The rest of the characteristics are the same as for the most detailed variant described in Section 3.4.2.

3.5.4. MO models without heat storage

MO models without heat storage are also a simplification of the most detailed MO model. In this case, the module for heat storage is not included. The rest of the characteristics are the same as for the most detailed variant described in Section 3.4.2.



Fig. 9. Strategy of the MO model to find the most economical solution.

4. Results

4.1. Comparison of MILP and MO models

Fig. 11 shows the heat and power generation by technology calculated with the MILP model, i.e., the reference scenario. In the reference scenario, heat generation in SA1 slightly reduces during the period 2030–2050 because of an improved energy efficiency in buildings [4]. Simultaneously, as prices of natural gas, electricity and CO₂ rise during this period, generating power becomes more costly, and power generation by CHP power plants decreases. Heat generation by CHP plants also reduces and is substituted by heat generated by other technologies, such as electric boilers (P2H). Other technologies are expected to play an important role in this scenario but without dramatic variations throughout the period of analysis, for example heat from third party integration (TPI), geothermal heat supply and biomass heat-only boiler (HOB).

A comparison of the heat and power generation across the different models is shown in Fig. 12. On the power generation side, all the different MO models follow the same reduction trend as the MILP model during the period 2030–2050. However, significant differences can be found across the different MO models. While annual percentage differences of $\pm 5\%$ vs. MILP are found in the most detailed MO model (Variant 1), differences of up to -40% are found in the MO models not considering CHP flexibility and up to $+18\%$ in the MO models considering flexibility but excluding heat storage. This suggests that excluding CHP flexibility results in an underestimation of power generation, while including flexibility but excluding heat storage results in an overestimation of it. Disaggregating these differences by technology (see Fig. 13) further reveals that MO models without CHP flexibility do not only underestimate CHP power generation, but also overestimate the conversion of electricity into heat in electric boilers. On the contrary, excluding heat storage underestimate the use of electricity in electric boilers.

On the heat generation side, all MO models generate the same amount of heat as the reference MILP model, which is expected, as the demand should be covered. Differences across models against MILP are only evident once they are disaggregated by technology, see Fig. 13. Results show that the MO model with CHP flexibility and heat storage offers annual percentage differences of up to $\pm 4\%$ against the reference

(Variant 1). This model slightly overestimates the heat generation by gas-fired heat-only boilers and proportionally underestimates the heat generation by CHP plants and electric boilers. These differences grow up to $\pm 10\%$ in the MO models excluding CHP flexibility (Variants 3 and 4). These models substantially underestimate the heat generation of CHP plants (e.g., gas-fired CHP and also TPI), while overestimating that of gas-fired heat only boilers and electric boilers. For the MO model including CHP flexibility but excluding heat storage (Variant 2), the differences grow up to 9%. This model overestimates heat generation by heat-only boilers and underestimates electric boilers, biomass-fired boilers and geothermal. This highlights the importance of heat storages to exploit the maximum potential of low-carbon technologies like biomass-fired HOB and geothermal, as well as sector-coupling technologies like electric boilers.

In other words, these results show that the MO model with CHP flexibility and heat storage (Variant 1) can explain $\sim 95\%$ of the heat generation effects and $\sim 93\%$ of the power generation effects estimated by the reference MILP model. MO models with either CHP flexibility or heat storage can explain $\sim 90\%$ of those effects, while MO models without any of these features can only explain $\sim 85\%$ of the effects.

The heat costs by technology for all scenarios are also calculated and compared. These are calculated as the marginal cost multiplied by the corresponding heat generation. For computing these costs, revenues obtained from power generation are included, but revenues obtained from heat generation are not. Since revenues from heat generation are the same for all the models, they do not influence the differences between the MO models and the reference. The percentage difference in heat costs for the different MO models compared to the MILP model are shown in Fig. 14. Results show that the differences in heat costs vs. the MILP model vary substantially depending on the MO model. In most of the years, the most detailed MO model presents net differences in heat costs of up to 10% vs. the MILP model on an annual basis, with one year exceeding 30%. In this model, heat costs of gas-fired boilers are overestimated, while heat costs of gas-fired CHP and P2H are underestimated. For the MO model excluding CHP flexibility and storage, differences range between 40 and 100%. In this model, heat costs of gas-fired CHP and boilers are largely overestimated, while heat costs of TPI and biomass boilers are significantly underestimated. A similar behavior, but with a much smaller difference (20–60%), is observed for the models considering either storage or CHP flexibility. Here again,

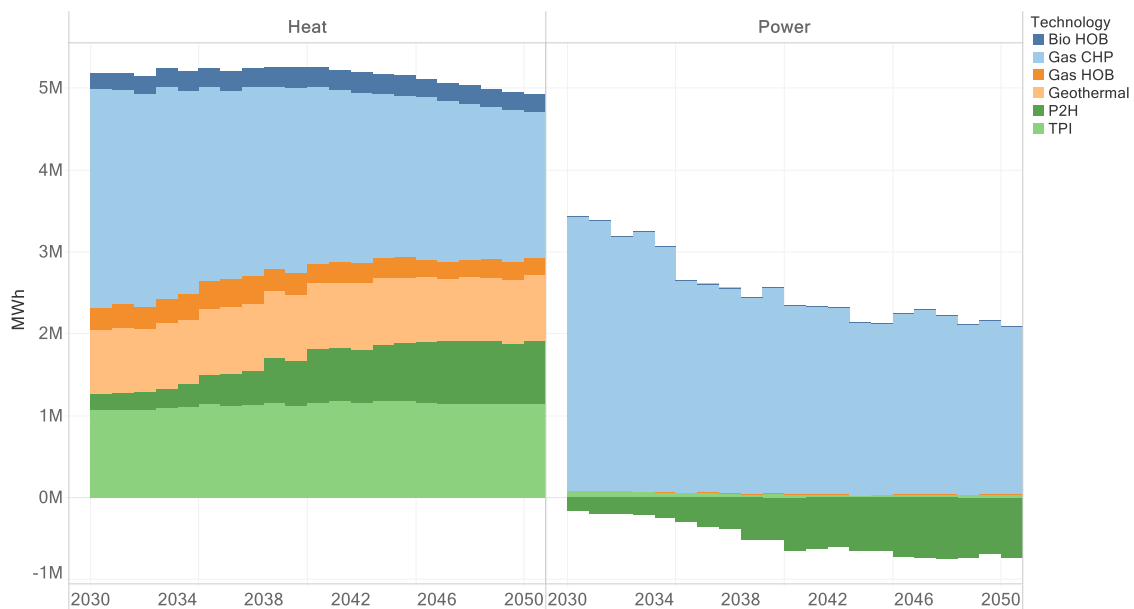


Fig. 11. Heat and power generation in MWh by technology for the MILP model.

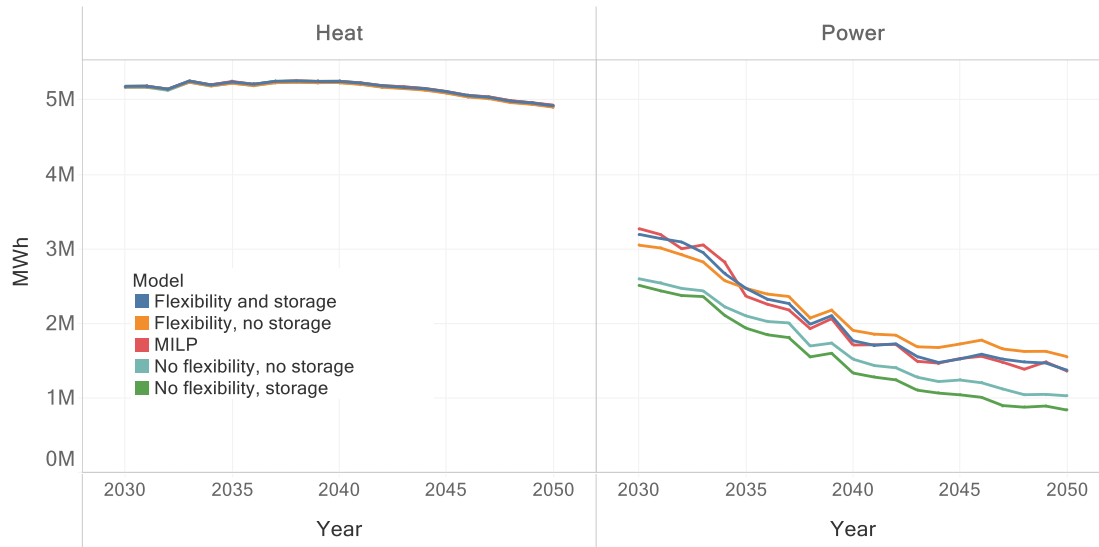


Fig. 12. Comparison of the heat and power generation in MWh for the different models.

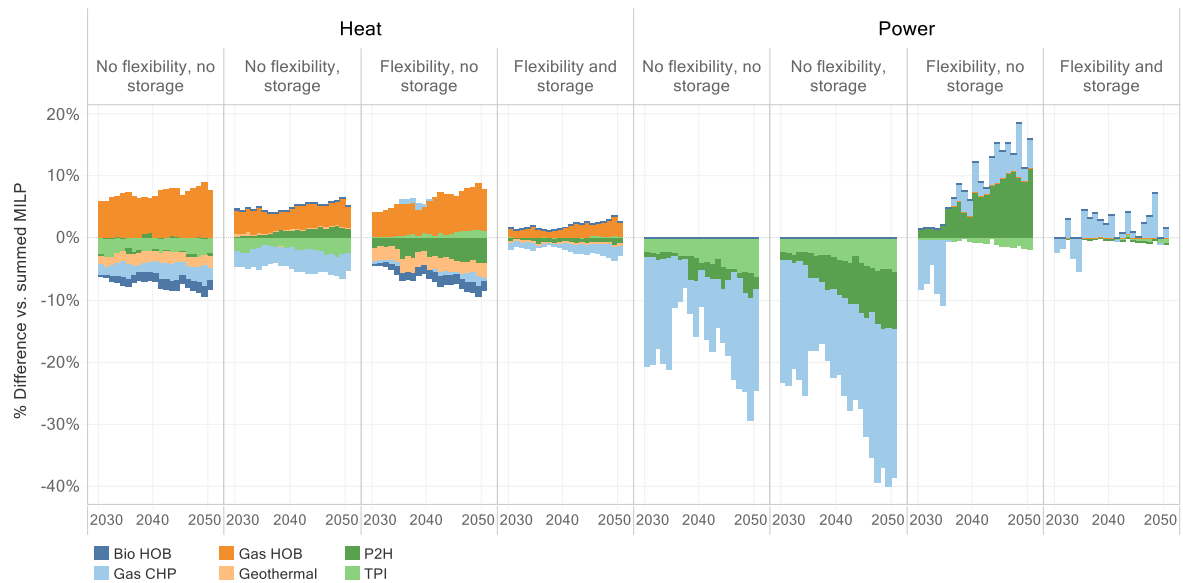


Fig. 13. Percentage difference in heat and power generation for the different MO models vs. MILP (annual aggregated values), disaggregated by technology.

heat costs of gas-fired boilers continue being overestimated and of P2H slightly underestimated.

To account for the overall difference in financial terms of the different MO models vs. the MILP model, the net present value (NPV) of the heat costs shown above is evaluated. Heat costs during the period 2030–2050 are converted to a present value, which is assumed to be year 2030. For calculating the NPV, the following equation is used:

$$NPV = \sum_{t=0}^N \frac{N_t}{(1+i)^t} \quad \text{Eq. 11}$$

where N_t is the net cash flow, i.e., cash inflow – cash outflow; i is the discount rate, which here is assumed to be 10%; and t is the time period of the cash flow. These results are then compared to the MILP model and the percentage difference is calculated.

Moreover, to have an indication of the computational intensity associated to the difference in NPV, the calculation time for all models is

also measured. Fig. 15 shows the percentage difference in NPV compared to the reference MILP model against the associated computational time.

Results suggest that the MO models offer a substantial reduction in computational time, at the expense of a reduction in the accuracy of the results that varies across models. MO models can reduce the computation time by almost three orders of magnitude compared to the MILP model, while achieving differences in NPV ranging from –6% for the most detailed MO model up to 25–50% for less detailed models. Computation times for the MO models can be considered conservative and subject to further improvement, as they were calculated in a computer less powerful (32 GB of RAM, 4 processors) than the one used to run the MILP models (128 GB in RAM, 24 processors). These results also suggest that it is necessary to include CHP flexibility and heat storage to minimize the differences against MILP models. In order to reduce this difference even further, it would be necessary to address the different features not included in the proposed MO model, namely the heat

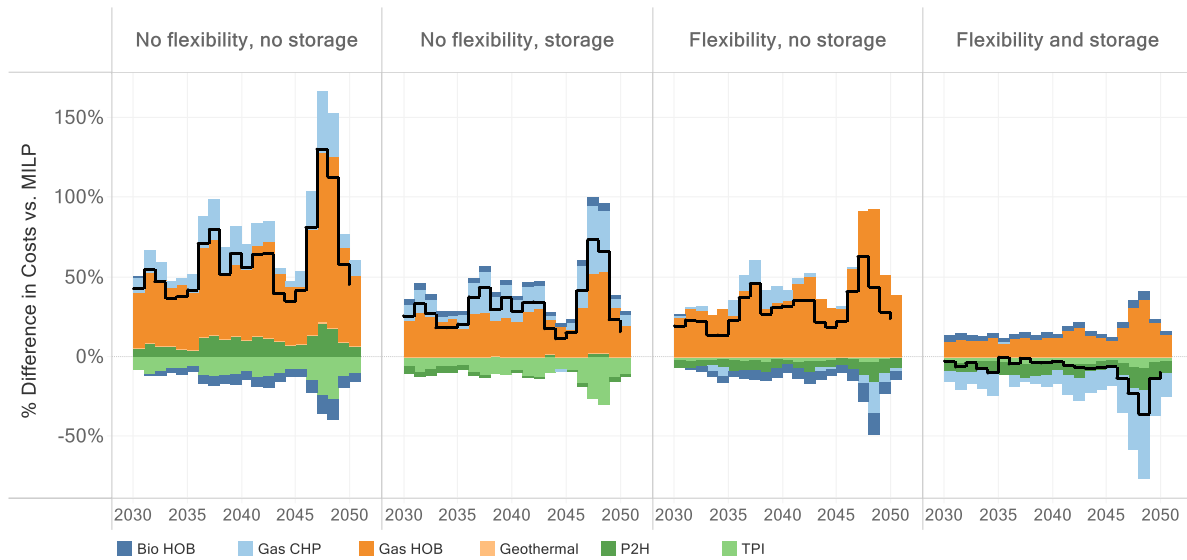


Fig. 14. Percentage difference in heat costs for the different MO models vs. MILP (annual aggregated values), disaggregated by technology. Black lines represent the net differences.

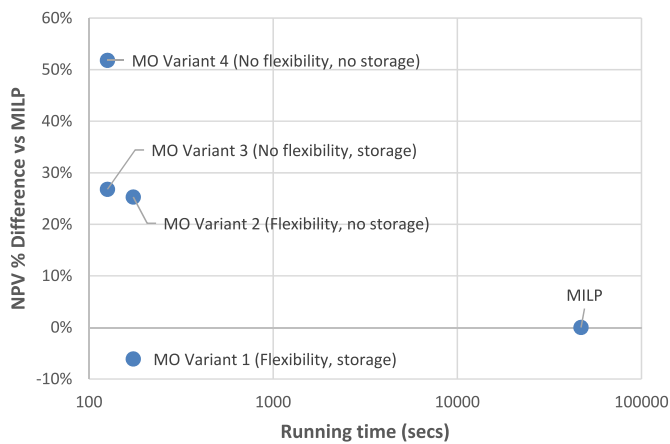


Fig. 15. Percentage difference in NPV vs. computation time.

transfer between sub-grids, and the variation in the supply and return temperature of the network.

4.2. Combination of MILP and MO models

Long-term portfolio optimization in the context of complex district heating and CHP systems demands high accuracy and high computational speed. However, as the presented results suggest, MILP and MO models offer one or the other but not both desired features at the same time. A relevant question, is whether a combination of these two methods could bring the best of the two worlds. We perform a simple experiment based on the results presented in the previous section. We evaluate the potential benefits of combining the two methods when a large number of runs is necessary, for example investment planning, e. g., finding the system capacity that ensures the highest NPV. While including the optimal system design in the objective function of the existing dispatch-optimization MILP model is possible (at expenses though of a large increase in computation time [60]), this option is unfortunately not available in the current version of BoFiT. To overcome this limitation, the approach is to run MILP and MO multiple times, each time with a different fixed capacity and then heuristically finding the

option with the highest NPV. While this approach does not guarantee a global optimum, it offers a pragmatic indication of superior technology mixes. We estimate the overall calculation time for the MILP model, the most accurate MO model (Variant 1) and a combinations of them. For the combination, the MO models are firstly run in full length and then a number of best alternatives is pre-selected and then separately re-run using MILP. Finally, the alternative with the highest NPV is identified. The number of pre-selected alternatives based on MO varies between 10, 20 and 50. Results are shown in Fig. 16.

The computation time for MO and MILP models is proportional to the number of runs. One thousand runs would take two days using the MO model and 550 days using the MILP model. Thus, using the MILP model alone (in the current BoFiT version) for investment planning is time prohibitive. The combination of the MO and MILP models is however advantageous. For a thousand runs, computation time would range from 7 to 29 days, depending on the number of pre-selected alternatives. For 10,000 runs, the computation time would increase to 31–47 days. These simple results show that combining MO and MILP models offers high speed and high accuracy, especially when a large number of runs might be necessary.

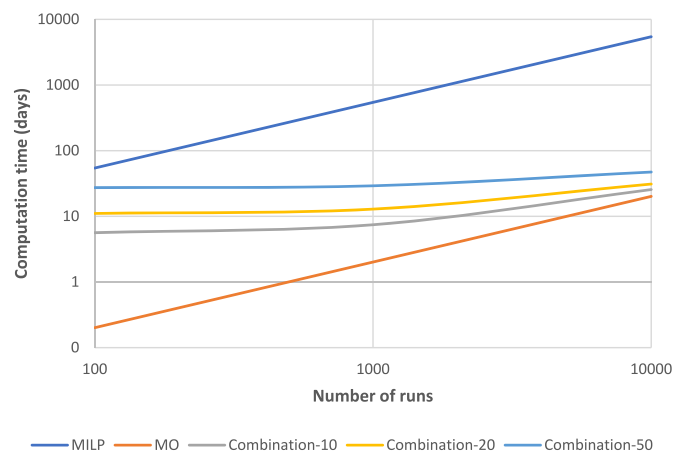


Fig. 16. Number of runs vs. computation time for MILP, MO and combinations.

5. Discussion

A state-of-the-art MILP model and various MO models with different levels of complexity were developed and used to optimize the portfolio of assets that serve a large portion of the district heating network in Berlin. The comparison was not intended to be mathematically exhaustive, but rather exploratory and aimed at finding alternatives to MILP that offer lower computational times and an acceptable accuracy.

Results suggest that for this study case, MO models with improved features have the potential to reduce calculation time compared to MILP models at the expense of a relatively low deviation in accuracy. In fact, MO models including CHP flexibility and heat storage have the potential to reduce calculation time by nearly three orders of magnitude compared to the state-of-the-art MILP models, while offering differences in heat generation and NPV of $\pm 4\%$ and -6% , respectively. While results are promising, it is important to say that they stand for the defined study case and further investigation is needed before extending these conclusions to other study cases.

In the context of district heating or CHP systems, a method that can speed-up calculations and maintain an acceptable level of accuracy can be critical to overcome several challenges. For example, MILP models are deterministic and typically do not consider uncertainties in assumptions because running many scenarios or performing stochastic optimization is time prohibitive. MO models could offer an advantage in this regard. Due to their faster calculation speed, MO models can perform many runs and thereby estimate how uncertainties in assumptions (e.g., price assumptions, weather assumptions, thermodynamic characteristics, etc.) influence the uncertainty of key parameters such as the NPV. A large number of runs that is not time-intensive could also be advantageously used to train machine learning models that allow the development of 'digital twins' of entire district heating networks.

Another potential application is the challenge of optimizing simultaneously the design and operation of an energy system. MILP methods can perform such optimization, but non-linear effects cannot be considered, including variation of the nominal efficiency of units as a function of size, variation of specific investment costs as a function of size, part-load performance, etc. [14]. While this problem can be solved using mixed integer non-linear programming (MINLP), iterative procedures [61] or multi-stage algorithms [62], these approaches are likely to increase computational resources. MO models evaluating the NPV and investment costs offer a key advantage. In this case, running a large number of runs through a Monte-Carlo algorithm could enable a heuristic optimization of the system design considering any non-linear effects in performance or investment.

However, MO models also pose various limitations. Firstly, their ability to consider some details of district heating networks is reduced. For example, their ability to model the variation of supply and return water temperatures in the district heating network as a function of the ambient temperature, as well as the hydraulic restrictions and heat transfer between sub-grids is limited. Secondly, their ability to describe details of the power plant performance is also limited, particularly the dependence of the performance on ambient conditions. While most of these limitations can be addressed by improving the algorithm, complexity would likely increase.

After considering the benefits and limitations of MO models described above, an important question is what role could MO models play for district heating or CHP applications. On the one hand, although their deviation is small in terms of heat generation, electricity and associated costs compared to the MILP reference, this small difference could lead to a wrong investment decision. This could be particularly true for those technologies that are over- or underestimated in MO models. On the other hand, MO models offer a superb speed that allows a new set of capabilities, ranging from exploring sensitivities or uncertainties to simultaneously optimizing the design and operation of the energy system. This could lead to a better understanding of design and operational risks and thereby improve the decision-making. To exploit

all the advantages and avoid the limitations of MO models, one possibility is to use them to complement MILP models. As shown in Section 4.2, MO models could be used prior to MILP models, to perform a pre-evaluation, an exploration of sensitivities or for downsizing the initial optimization problem. Once key solutions (e.g., technologies, parameters, ranges, etc.) are identified, they can afterwards be re-evaluated in MILP models to obtain a higher accuracy estimation. This approach could lead to faster and more robust decision-making.

6. Conclusions

This paper compares two modeling approaches for portfolio optimization in district heating, namely the state-of-the-art mixed integer linear programming (MILP) and the merit order (MO). While MILP is extensively used but also computing- and resource-intensive, MO offers a simplified approach that results in faster calculations. The key question is to what extent the simplified approach and higher speed of MO models implies a reduction in accuracy compared to MILP models. The comparison was not intended to be mathematically exhaustive, but rather exploratory and aimed at finding alternatives to MILP that offer lower computational times and an acceptable accuracy.

To address this challenge, we have firstly defined a study case to be evaluated with both methods. Supply Area 1 (SA1) of the district heating system in Berlin is selected, which is the largest in Germany and the third largest in the EU-27. Secondly, we have created a high-fidelity MILP model of the study case using the commercial software BoFIT, which finds the most cost-effective combination of technologies to meet demand and excludes investment optimization. The MILP model considers various important features of the district heating system, including i) a detailed depiction of the CHP units, ii) heat transfer between sub-grids, iii) supply and return temperatures of the district heating network and iv) heat storage.

Then, we have developed various MO models with different levels of complexity in order to identify which features have the most influence on the accuracy. MO models share some features with the MILP model but differ in others. MO models consider exactly the same technology portfolio and capacity restrictions of the grid as the reference MILP. However, while the reference MILP model optimizes the costs of the system and allows heat transfer between sub-grids, MO models perform the merit order optimization for each sub-grid and do not consider heat transfer between sub-grids. MO models do not consider either the variation in supply and return temperatures of the heat network. Furthermore, two features are considered differently across the proposed MO models: i) a detailed depiction of CHP plants and ii) inclusion of heat storage. Key measures to compare the different models include the heat and power generation, the associated heat generation costs, the sum of the discounted heat generation costs (i.e., the net present value) and the calculation time.

Results suggest that MO models including heat storage and describing CHP plants in detail have the potential to reduce calculation time by nearly three orders of magnitude compared to the reference MILP model without significantly sacrificing accuracy. In fact, differences in heat generation by technology and NPV account for $\pm 4\%$ and -6% , respectively. While results are promising, it is important to say that they stand for the defined study case and further investigation is needed before extending these conclusions to other study cases.

An important question is what role could MO models play for portfolio optimization of district heating or CHP applications. Results show that combining MO and MILP models is advantageous and offer high speed and high accuracy, especially when a large number of runs might be necessary. For example, MO models could be used prior to MILP models to perform a pre-evaluation, an exploration of sensitivities or for downsizing the initial optimization problem. This could reduce the number, or the extension of otherwise lengthy MILP runs. Once key solutions are identified, they can afterwards be re-evaluated in MILP models to obtain a higher accuracy estimation. Thus, combining MO and

MILP models for long-term portfolio optimization could result in a faster and more robust decision-making, which could otherwise not be attained with any of the two options individually. The presented results can provide guidelines for similar studies addressing the challenge of optimizing the operation and design of district heating networks or CHP units in other cities or regions with comparable decarbonization goals.

Credit author statement

M. Gonzalez-Salazar: conceptualization, methodology, development of MO models, data analysis, writing and editing. J. Klossek: methodology, development of MO models, data analysis, editing. P. Dubucq: methodology, development of MO models, editing. T. Punde: development of MILP models. All authors have read and agreed to the published version of the manuscript.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data that has been used is confidential.

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