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Environmental impacts of aquifer thermal energy storage (ATES)

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ABSTRACT

Aquifer Thermal Energy Storage (ATES) is an open-loop geothermal system allowing long-term storage of thermal energy in groundwater. It is a promising technology for environmentally friendly energy generation that can reduce greenhouse gas (GHG) emissions. In the literature, there are few studies on the greenhouse gas emissions caused by ATES systems over their entire life cycle. Thus, this study presents a novel life cycle assessment (LCA) regression model that can be used for a wide range of ATES configurations due to its parametric structure. This model is a fast alternative to conventional time-consuming LCAs. Combined with a Monte Carlo simulation, it enables the analysis of the environmental impacts of a large variety of hypothetical ATES systems and therefore the evaluation of the technology as a whole. Compared to conventional heating systems based on heating oil and natural gas, the median value of the Monte Carlo simulation results in GHG savings of up to 74%. In comparison to cooling techniques using today's electricity mix, ATES can save up to about 59% of GHG emissions, while also being economically competitive. When considering a projected electricity mix for the year 2050, the GHG emission savings resulting from a second LCA regression model are as high as 97%. The findings of our sensitivity analysis show which ATES design parameters should be optimized when planning new systems. In particular, the most important design parameters *operating time cooling* and *coefficient of performance* (COP) of the heat pump should be carefully considered.

1. Introduction

Aquifer Thermal Energy Storage (ATES) is a technology for long-term storage of thermal energy using groundwater. These open-loop geothermal storage systems take advantage of the high heat capacity of groundwater and its large volumes that are widely available [1,2].

Typically, ATES systems are used for large-scale applications due to their high storage capacities. Exemplary use cases of ATES systems are the heating and cooling supply of office buildings, hospitals, airports or universities. ATES has also been deployed for supply of district heating networks [3,4]. Suitable hydrogeological conditions are required for the application of ATES, including a highly permeable aquifer and low groundwater flow velocities, among others [4].

Climatic factors are also relevant for an efficient use of ATES. Particularly in regions with a moderate climate and distinct seasonal temperature differences ATES is well suited to mitigate the seasonal mismatch between the availability and the demand of heating and cooling energy to supply buildings [3–7]. Similar to ground source heat pump (GSHP) systems, it is therefore a promising technology for environmentally friendly energy generation that can reduce CO_2 emissions [8,9].

ATES systems are based on the long-term creation of a warm and a cold storage volume in the subsurface. Depending on the heating or cooling demand, the groundwater can be extracted from the corresponding storage volume to supply the buildings with energy. Typically, in heating mode a heat pump is used whereas with cooling mode a so-called direct cooling loop without using the heat pump is often designed [2,4]. The vast majority of ATES systems are classified as low-temperature-ATES (LT-ATES) with maximum injection temperatures of below 25 °C and are usually using shallow groundwater of the upper few tens to hundreds of meters [3,10,11].

More than 2800 ATES systems have been successfully implemented worldwide [4]. Most of these systems are located in the Netherlands,

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Abbreviations

ATES	Aquifer Thermal Energy Storage
COP	Coefficient of Performance
CO_{2eq}	Carbon dioxide equivalents
GHG	Greenhouse Gas
GSA	Global Sensitivity Analysis
GSHP	Ground Source Heat Pump
GWHP	Groundwater Heat Pump
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LT	Low Temperature
MC	Monte Carlo

which is characterized by suitable climate and underground conditions with a predominantly homogeneous subsurface with slow groundwater velocities. There are ongoing efforts to find similar conditions in other countries in favour of ATES [7,12–14]. However, to pave the way for an increasing spread of the technology, a main determinant is also its environmental performance such as the capability to reduce greenhouse gas (GHG) emissions.

Life Cycle Assessment (LCA) is a common and standard method to evaluate GHG emissions and other environmental impacts of technologies [15–18]. Until now, comprehensive LCAs that evaluate the GHG performance of ATES systems are scarce. Tomasetta [19] and Tomasetta et al. [20] conducted an LCA of a Dutch ATES system consisting of two boreholes reaching to a depth of 80 m. However, in contrast to the common bimodal ATES application for heating and cooling only the heating was investigated. Its heating capacity is stated as 250 kW with an annual full-load operation time of 2000 h. A main finding is that the Dutch system has considerably lower environmental impacts than a conventional heating system such as a natural gas boiler. Unfortunately, no specific numbers for possible reductions of GHG emissions are provided.

The LCA in the study by Moulopoulos [21] also refers to a Dutch ATES system again consisting of two wells that supply an office building complex with an approximate area of 6000 m^2. It is used for combined heating and direct cooling operation and thus complies with the typical ATES utilization scenario. In heating mode, a heat pump is required that is supported by a natural gas boiler. The LCA is based on a data survey presented as a Life Cycle Inventory (LCI) and its results are divided into several life cycle phases. The author also states that the described ATES system can save up to 45% of GHG emissions compared to a conventional heating and cooling system. Due to the LCA's inclusion of an elaborate waste water treatment, it can be assumed that these savings are lower than for a typical ATES system without incurring waste water.

Ni et al. [22] carried out two LCAs for comparing an ATES system with a conventional heating and cooling system that are both situated at a hypothetical location in China. A special feature investigated in this study is the combination of both technologies with in-situ bioremediation using a biological medium containing dechlorinating bacteria that is added into the aquifer. As stated in Ref. [22], the thermally altered subsurface in case of ATES should enhance the bioremediation effect. The result of the comparison of both LCAs is a considerably lower environmental impact for ATES and bioremediation. Over all impact categories, it is about 50% less than for the conventional system and bioremediation. Regarding the GHG emissions, the ATES produced about 67% less CO_{2eq}. A sensitivity analysis conducted for the ATES investigates various life cycle stages such as material acquisition, construction and operation. It revealed that the system operation is the most important stage. A detailed sensitivity analysis of individual system design parameters like ATES capacity or well depth was however not performed. Furthermore, the combination of ATES with in-situ bioremediation is a very uncommon application that is not representative of the typical and standard ATES use.

Thus far, the limited work available in this field is insufficient for assessing the environmental potential of ATES in a rigorous manner. Our study aims to generally assess the GHG emissions of ATES systems and possible GHG savings compared to conventional heating and cooling systems. We therefore refer to a real application that serves to carry out LCAs for many different hypothetical ATES systems defined by varying combinations of characteristic parameters. The execution of a detailed LCA study – especially the collection of reliable input and output data during the LCI – is a time-consuming process and it may not be possible to consider all the uncertainties, especially those of geological parameters. This study presents a way to carry out LCAs of ATES systems in a streamlined and time-saving way, concentrating on the systems' GHG emissions. An LCA regression model enables a quick execution of a large number of LCAs by including only a limited number of variable input parameters. This provides a fundamental knowledge base for a more comprehensive evaluation of the ATES technology in terms of environmental performance. The median value of a Monte Carlo (MC) simulation is considered as a typical ATES system which is used to determine possible GHG savings achievable by the technology when compared to conventional heating and cooling systems. Furthermore, the most influential parameters regarding GHG emissions are identified by using a global sensitivity analysis (GSA). This enables for a targeted optimization of existing and planned ATES. The underlying idea for the selected workflow originates from Padey et al. [18] and Lacirignola et al. [16], who presented LCAs for wind power and enhanced geothermal systems (EGS), respectively. In addition, results from previous studies on the economic performance of ATES systems are reviewed in order to evaluate the overall benefits of this technology in comparison to conventional energy systems.

2. Materials and methods

2.1. Study site

Although, a substantial potential of ATES was shown for Germany [23], only a small number of systems have been realized due to the technology's low level of awareness and legislative barriers [4,24]. Being one of the few German systems, an LT-ATES has been in operation at the "Bonner Bogen" area since 2009 supplying a hotel with a congress center, office buildings, a data center and a medical center (Fig. 1). The system is one of Europe's largest heat pump systems with an authorized flow rate of up to 1,455,000 m^3/a. Here, six wells with a maximum depth of about 28 m are used for the heating and cooling supply of a useable area of around 60,000 m^2 (Table 1). In the cold season, a heat coverage of 60%–80% is achieved using the water from the warm storage in combination with heat pumps. Two gas boilers are available to cover peak loads during very low outside air temperatures [25]. In summer, the water circulation is reversed in order to extract the cold groundwater allowing for the area's direct cooling supported by refrigeration machines. The year-round cooling of the data center causes an increased cooling demand at the site resulting in an elevated heat input into the aquifer. Further constructional and operational details of the "Bonner Bogen" ATES are given in the Table 1.

2.2. Life cycle assessment

Life cycle assessment (LCA) is a standardized methodology to determine the environmental impacts of products, processes or technical systems (ISO norms 14040 and 14044) [26,27]. A LCA study is based on the establishment of an LCI including all inputs (materials, processes, etc.) and outputs (e.g. energy as heat and cold) that are required or produced during the considered life cycle from a 'cradle to grave' perspective. Within an LCA, environmental impacts are allocated from

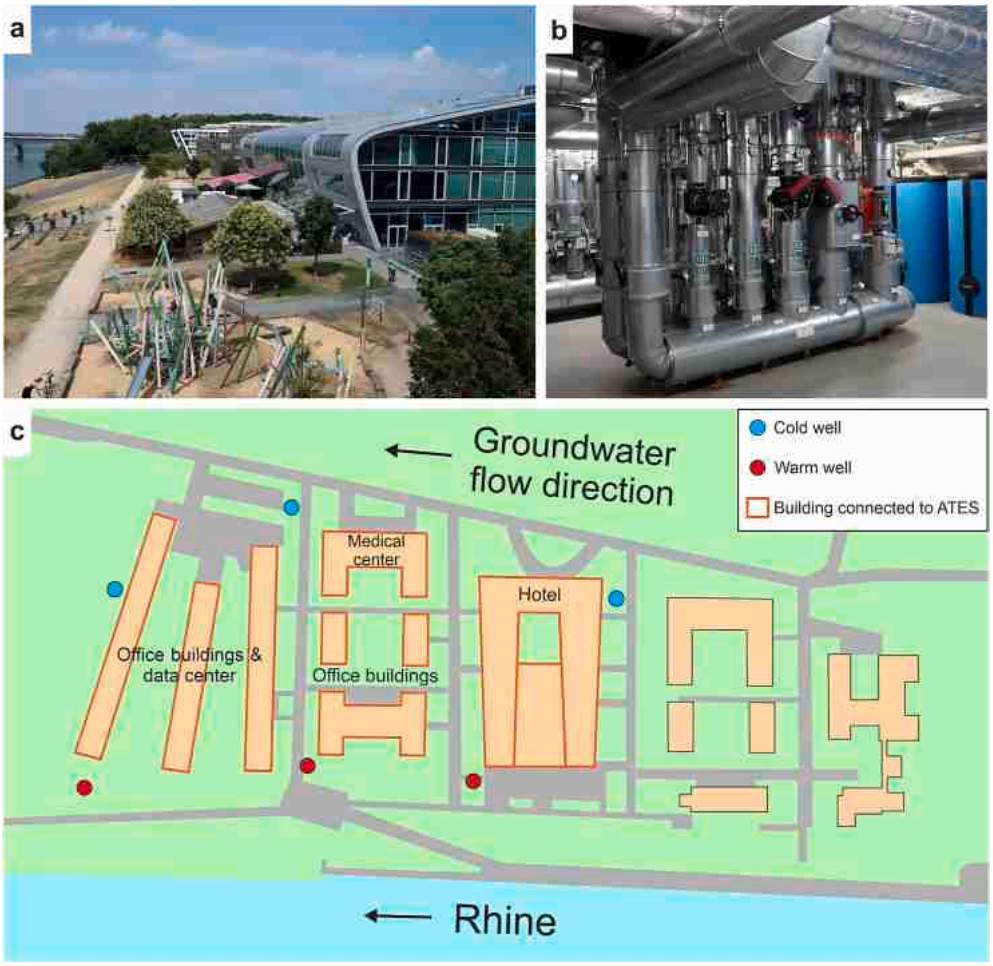


Fig. 1. Impressions of the ATES site "Bonner Bogen": Hotel building connected to the ATES (**a**) and technical center of the aquifer storage system (**b**). Fig. **c** shows a site map of the "Bonner Bogen".

Table 1
Main characteristics for the LCA of the ATES system at the "Bonner Bogen".

	Parameter	Value	Unit	Source
Subsurface	Depth of boreholes	22–28	m	[25]
	Number of boreholes	6	–	[25]
	Energy demand of the submersible pumps[a]	167.6	MWh_{el}/a	EcoVisio GmbH
Surface	Installed capacity[b]	–	MW_{th}	
	Energy demand of the heat pump[a]	808.1	MWh_{el}/a	EcoVisio GmbH
Operation	Maximum production rate	300	m^3/h	EcoVisio GmbH
	Heat production[a]	2164	MWh_{th}/a	EcoVisio GmbH
	Cold production with heat pump[a]	3188	MWh_{th}/a	EcoVisio GmbH
	Direct cold production[a]	812	MWh_{th}/a	EcoVisio GmbH

[a] The given values refer to the year 2016.
[b] No information available. Instead, the base case LCA of the ATES system at the "Bonner Bogen" was conducted using the provided numbers for heating and cooling.

the LCI data to impact categories by means of an impact assessment.

The main focus regarding the LCA in the present work is on the system's GHG emissions in relation to the amount of heating and cooling energy provided by the system. Hence, the functional unit of the LCA is 'gCO_{2eq}/kWh_{th}'. Establishing this functional unit allows a comparison between ATES and other heating and cooling technologies. The ATES system boundaries regarded in the LCA reach from the groundwater conditions over the subsurface construction to the heat pump. The buildings' energy distribution system connected to the aquifer storage is not included as it is a basic requirement regardless of the energy system.

2.2.1. *Life cycle inventory*

The base case LCA model used as a foundation for the developed LCA regression model examines the environmental impacts of the ATES system at the "Bonner Bogen". The LCI of the base case LCA model is subdivided into five related life-cycle stages: (1) well construction, (2) surface construction, (3) subsurface construction, (4) operation and (5) decommissioning. The life-cycle stage 'well construction' consists of the construction materials and processes for well drilling, well piping and well development as well as construction of the well chamber.

A complete compilation of the LCI is presented in detail in the Supplementary data (Section SD1). The input and output components are

collected from the ecoinvent 3.5 database [28,29]. For each component, the listed amount is related to one well. Due to the uniform depth of all six wells at the site, the total amounts can be calculated by multiplication. The amount of each material or process is derived or calculated from manufacturing specifications and considering the constructional details such as borehole depth or size of the well chamber. Underlying information was provided by the two companies EcoVisio GmbH and Knauber Contracting GmbH, which are responsible for planning, realization and operation. Regarding the LCI entries, several assumptions and estimations had to be made where no constructional and operational details were available. These are based on literature information (e.g. Ref. [30]) or comparable projects (e.g. Aquadrom Hockenheim, Germany) (Supplementary data, SD2).

The uncertainties specified in the Supplementary data (SD1) are mainly caused by the absence of precise specifications regarding some constructional or operational details. Furthermore, in some cases there are no items in the LCI database that are able to exactly represent the situation on site. In these cases, the most appropriate database product or process was chosen.

2.2.2. Life cycle impact assessment

Within an LCA, the allocation of quantified environmental impacts to each LCI item is done during the life cycle impact assessment (LCIA) phase. Here, characterization factors are applied to all input and output data collected in the LCI. The characterization results are then aggregated to various impact categories according to the used impact allocation method providing the characterization factors [17].

The impact allocation method used in this study is IMPACT 2002+ V2.10 [31]. The main focus of the present work is on the systems' GHG emissions represented by the impact category 'climate change' (functional unit: gCO_{2eq}/kWh_{th}). However, the base case "Bonner Bogen" LCA model was also evaluated for the additional impact categories 'human health' ($DALY/kWh_{th}$) covering human toxicity and respiratory effects and 'ecosystem quality' ($PDF \times m^2 \times yr/kWh_{th}$) referring to aquatic acidification and aquatic eutrophication. Furthermore, it was evaluated for the category 'resources' ($kJ\ primary/kWh_{th}$) such as non-renewable energy consumption [31]. Similar to the compilation of the LCI, the impact assessment was carried out with the LCA software SimaPro (Version 9.0.0.35) using the above-mentioned allocation method.

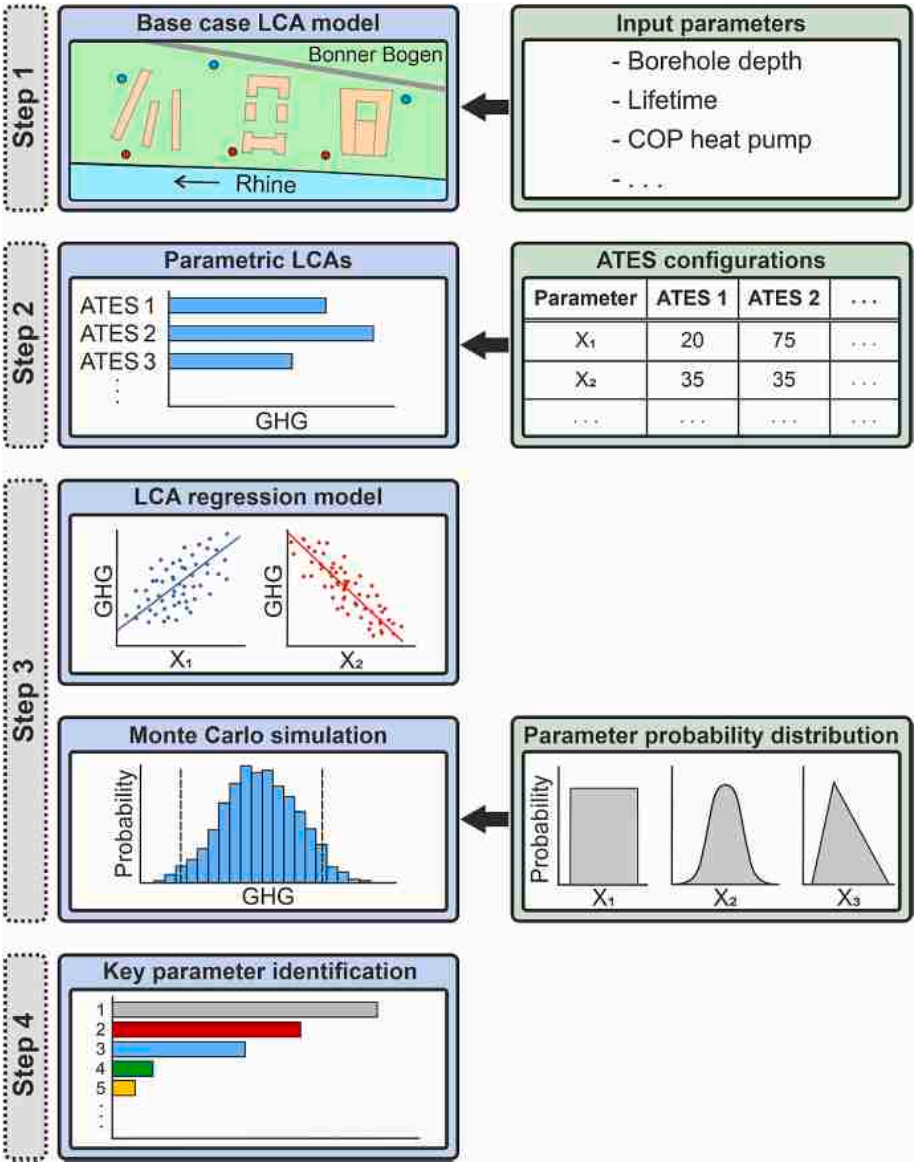


Fig. 2. Workflow for creating the LCA regression model for ATES systems.

2.2.3. Interpretation

The interpretation phase of an LCA aims for delivering results relevant to the defined goal and scope of the study. This is done by a combined consideration of the inventory analysis and the impact assessment. Thus, the interpretation phase serves the purpose to provide understandable and consistent conclusions able to explain limitations and to derive recommendations.

2.3. Creation of the LCA regression model

The workflow for generating the LCA regression model can be divided into the following steps (Fig. 2):

Step 1: Creating the base case LCA model at the "Bonner Bogen" including selected input parameters that define the system configuration.

Step 2: Parametric LCAs of 70 hypothetical ATES configurations using the LCA model.

Step 3: Design of the LCA regression model and generation of an ATES GHG distribution profile using Monte Carlo (MC) simulations.

Step 4: Identification of important key parameters by means of a global sensitivity analysis (GSA).

The workflow presented in this study is adapted from the studies by Padey et al. [18] and Lacirignola et al. [16].

2.3.1. Base case LCA model

While the base case LCA model of the ATES at the "Bonner Bogen" is site-specific for this system's configuration, the independent variation of ten included system-characterizing parameters allows the model's application to a wide range of different ATES configurations. Accordingly, the included parameters function as scaling factors to adjust the amount of LCI items (e.g. amount of filter gravel, length of electrical cables, fuel needed for drilling) that were initially specified for the study site (see also Supplementary data, SD1). The selected parameters represent characteristics generally required to describe the dimension, construction and operation of an ATES system. The parameter *COP heat pump* does not only represent the operation conditions of the building heating system that is connected to an aquifer storage, but serves as an indicator for the overall performance of the ATES systems' subsurface components including effects of underground heat loss.

Table 2 provides an overview of the ten included parameters and the respective ranges within which they can be varied. Based on information from literature, a probability distribution for each parameter is specified for use in Monte Carlo (MC) simulations (Table 2). Also, mathematic independence of the model parameters is a necessary condition that allows for the correct application of the global sensitivity analysis which has to be conducted to identify the key parameters in the last of the above listed steps.

Table 2
Input parameters included in the LCA model.

Parameter	Symbol	Unit	Characteristic value	Probability distribution	Main references
Depth of boreholes	*d*	m	185	Uniform (20, 350)	[4]
Flow rate (whole system)	*fr*	m^3/h	365	Uniform (10, 720)	[4]
Number of wells	*Nw*	–	2	Half-normal (2, 64)	[4]
Fuel for drilling	*fd*	t/m	0.12	Uniform (0.07, 0.16)	[16]
Operating time heating (full load equivalent)	*Th*	h/a	2500	Uniform (1500, 3500)	[2,32]
Operating time cooling (full load equivalent)	*Tc*	h/a	1600	Normal (1600, 4×10^6)	[33]
Lifetime	*L*	a	35	Normal (35, 25)	[34,35]
Specific power of well pumps (per pump)	*Pp*	kW/(l/s)	0.6	Uniform (0.3, 0.9)	[36,37]
COP heat pump	*COP*	–	3.5	Triangular (3, 3.5, 7)	[38,39]
ATES capacity	*Cap*	kW	2000	Uniform (200, 2×10^4)	[4]

2.3.2. Parametric LCAs

In order to create the LCA regression model, the parameterized LCA model is used to evaluate the environmental impacts of 70 dissimilar ATES configurations. Each hypothetical ATES system corresponds to a different combination of the ten parameters listed in Table 2. The generation of the 70 parameter sets is done following a one-at-a-time (OAT) approach, thus only one parameter is changed at a time, while all other parameters are kept at their characteristic values (arithmetic mean, expected value or mode). Each of the ten parameters is varied in seven equidistant steps within its respective range leading to a total number of 70 different parameter sets and associated LCA results.

2.3.3. LCA regression model

Using the 70 LCA results obtained with the parameterized LCA model, a multiple linear regression analysis is conducted in order to create the LCA regression model. It aims to quantitatively describe the LCA results in the form of GHG emissions as a function of the ten system-specific parameters from Table 2. The regression model follows a simple linear form:

$$GHG_{ATES}\left[\mathrm{gCO_{2eq}} \,/\, \mathrm{kWh_{th}}\right] = \alpha_0 + \sum_{i=1}^{n} \alpha_i X_i \quad \text{, where n} = 10 \tag{1}$$

Here, α_0 represents the regression constant and α_i the regression coefficients obtained from the regression analysis. X_i marks the ten included parameters. The regression analysis is conducted using the statistics software SPSS. More detailed information about the principles of multiple linear regression analysis can be found in Montgomery et al. [40].

Due to its simple form, the regression model can be used in a straightforward way in MC simulations to obtain the GHG emissions of 10,000 different ATES configurations. Again, each configuration consists of a unique combination of values of the ten input parameters that are randomly generated according to the respective probability

Table 3
Estimated shares of different types of energy of the utilized current German electricity mix (ecoinvent 3.5) and the projected German electricity mix in 2050.

Type of energy	Share of the current electricity mix[a] (%)	Share of the 2050 electricity mix [41,42] (%)
Lignite	26	0
Hard coal	20	0
Nuclear	17	0
Wind power – onshore	10	42
Natural gas	7	4
Imports	7	10
Biogas	6	0
Hydropower	5	3
Biomass	1	4
Wind power – offshore	0.3	19
Photovoltaics	0	18

[a] The German electricity mix provided in ecoinvent 3.5 refers to the year 2014. A more recent mix is not available in the LCI database.

distribution from Table 2. In this way, the GHG emissions from a large variety of possible ATES systems can be evaluated making up for the lack of explicit LCA studies in literature. This panel of GHG emission results obtained with the MC simulation is also compared to specific LCA results published in the literature to verify the robustness of the LCA regression model.

In addition, a second regression model is created to evaluate the impact of a different electricity mix on the overall GHG performance of ATES systems over their lifetime. This second model is also derived from the base case LCA model with a modified LCI considering the projected German electricity mix for the year 2050 with a significantly higher share of renewable energies (Table 3).

2.3.4. Global sensitivity analysis

The ten input parameters included in the LCA regression model (Eq. (1)) do not contribute equally to the variance of the model output, i. e. the GHG performance. Hence, a global sensitivity analysis (GSA) is performed to identify the key parameters that contribute the most to the model's output variance. In this study, the GSA is carried out using the Sobol method over a large sample of different ATES configurations. This method enables the calculation of estimated values for Sobol indices of first, higher and total order [18,43]. Here, the mathematical independence of the ten input parameters allows a complete variance decomposition and leads to a formulation of the total variance as a sum of the variance contributions of each individual parameter as well as their respective interactions with each other [43].

These parameter interactions are represented by the higher and total order Sobol indices. Due to the design of the regression model as a linear and additive model, no higher order parameter interactions are to be expected [44]. Thus, only the first order Sobol indices are calculated (see also Supplementary data, SD3).

3. Results and discussion

3.1. Environmental impacts

The results of the LCA model for the base case ATES system at the "Bonner Bogen" are shown in Fig. 3. The LCA model was evaluated for the four impact categories 'human health', 'ecosystem quality', 'climate change' and 'resources'. For each impact category, Fig. 3 also illustrates the share of the individual life cycle phases using the current German electricity mix (Fig. 3a) and the projected German electricity mix for the year 2050 (Fig. 3b). When using the current electricity mix, it is apparent that the operation of the ATES system is the dominating life cycle phase regarding the first three impact categories 'human health', 'ecosystem quality' and 'climate change'. The impact on 'climate change' which represents the GHG emissions is almost solely caused by the operation phase. A more detailed evaluation of the LCA results also reveals that within the operation phase, the electricity supply for running the ATES is the most influential factor (not shown in Fig. 3). Regarding the 'resources' category, it can be seen that the subsurface construction phase has the largest share in the overall impact of the study site. This is mainly due to the material demand in form of high-density polyethylene water pipes that were embedded into the ground.

If the projected 2050 electricity mix is considered, the share of the operating phase in the categories 'human health', 'ecosystem quality' and 'climate change' decreases while particularly the share of the subsurface construction phase increases. Regarding the 'resources' category, there are only minor changes and the subsurface construction phase still accounts for the largest share of this impact. A quantitative comparison between the LCA results using the different electricity mixes regarding the 'climate change' category is shown in Fig. 6.

Previous ATES studies found in the literature often present overall lifetime environmental impacts without a detailed comparison. Tomasetta [19] and Tomasetta et al. [20] focus on the relative environmental benefits of the considered ATES system compared to a conventional heating system (i.e. a natural gas boiler). Moulopoulos [21] also states that the operation phase is dominant in most impact categories

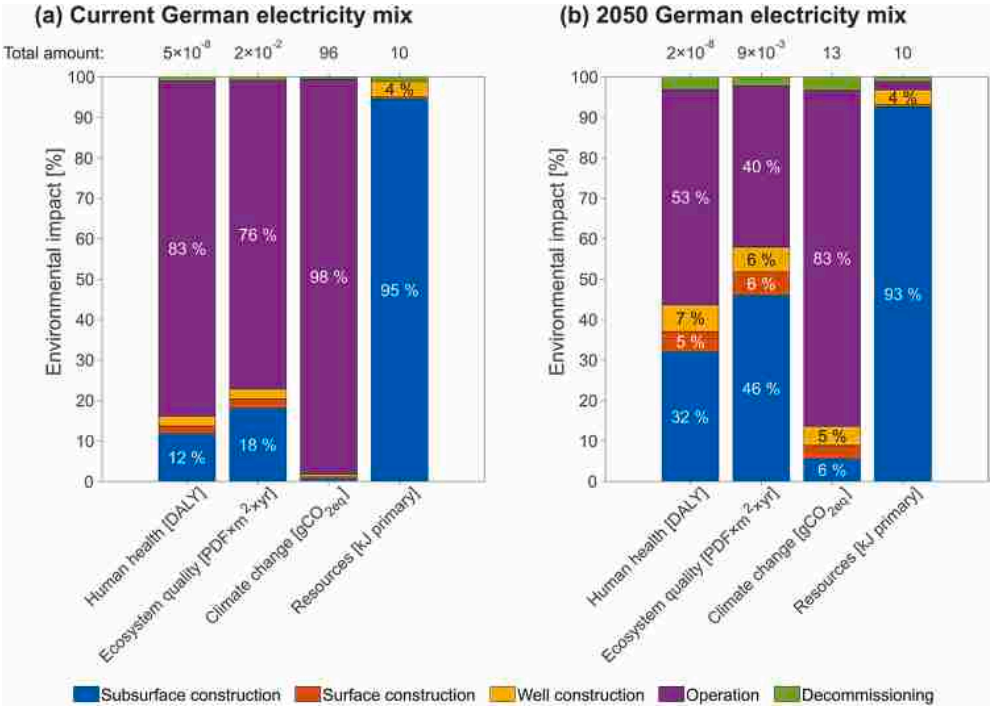


Fig. 3. LCA results per kWh_{th} of the base case scenario at the "Bonner Bogen" using the current German electricity mix (**a**) and a projected German electricity mix for the year 2050 (**b**).

including climate change, even though this LCA includes a waste water treatment within the end-of-life phase that is also influential regarding GHG emissions.

The most recent study performed by Ni et al. [22] is an LCA of a combination of ATES and in situ bioremediation. The results are presented with regard to a similar life cycle, yet refer to a different impact assessment method. Similar to the present study and the aforementioned studies, the authors demonstrated that the operation phase is by far the most impactful phase regarding climate change (here termed as global warming potential). The second most impactful life cycle phase across all impact categories in Ni et al. [22] is the material acquisition phase. It should be noted however that most of this impact is due to the production of the biological medium necessary for the in situ bioremediation and therefore not directly comparable to a standard ATES system without any bioremediation. A quantitative comparison with the results from previous studies is shown subsequently after the formulation of the regression model.

3.2. LCA regression models

Based on the design of the regression model for GHG emissions of the ATES systems in Eq. (1), the fully formulated LCA regression models referring to the current and the 2050 German electricity mix are obtained by means of a multiple linear regression analysis. The models are presented in the Supplementary data (SD4).

Fig. 4 illustrates the LCA results of the MC simulation from the regression models using 10,000 randomly generated ATES configurations. The blue dashed lines mark the median values of the distribution at 83.2 gCO_{2eq}/kWh_{th} when using the current German electricity mix (Fig. 4a) and at 10.5 gCO_{2eq}/kWh_{th} for the projected 2050 electricity mix (Fig. 4b).

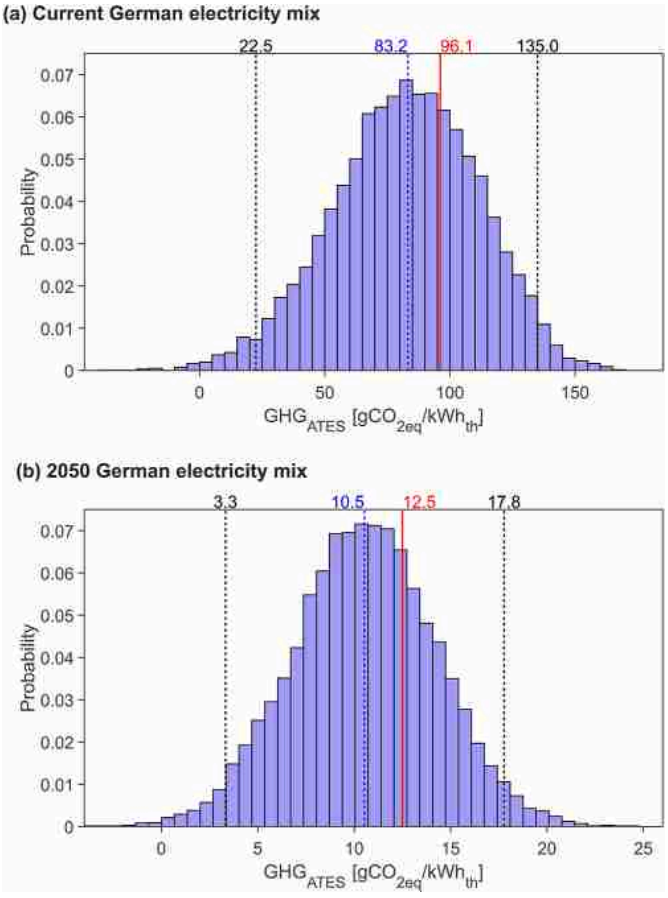
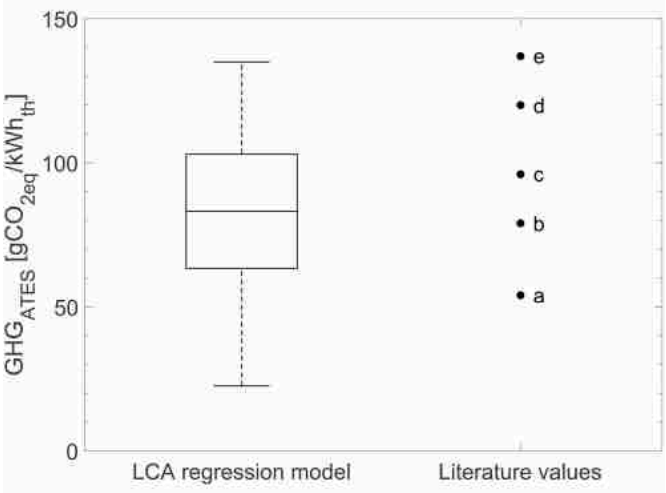


Fig. 4. Histogram of the results of the MC simulation using the LCA regression model based on the current German electricity mix (**a**) and on the projected 2050 German electricity mix (**b**). The blue dashed lines mark the median of each distribution. The red lines show the LCA results of the respective base case scenario at the study site "Bonner Bogen". Quantiles 2.5% and 97.5% are represented by black dashed lines.

The random generation of each of the 10,000 different parameter sets, i. e. ATES configurations, can sporadically lead to parameter combinations that are unlikely to correspond to a viable ATES system in terms of technical and economic feasibility. One example would be a parameter combination with both a very low ATES capacity and very high flow rate. The negative LCA results shown in Fig. 4a can be explained by these unlikely parameter combinations and the formulation of the regression model as a linear combination including both positive and negative coefficients. However, with far less than 1% of the total number of individual model runs during the MC simulation, the impact of the negative results on the overall MC result can be neglected. The LCA results of the unlikely parameter sets as well as the negative results are dealt with by disregarding statistical outliers below quantile 2.5% and above quantile 97.5% for the further analysis (Fig. 4). The unlikely parameter combinations described above could be suppressed by including mathematical relationships between the parameters, such as dependencies or mutual constraints. A suitable tool for this could be the use of copula functions in the regression models. However, there is currently not enough data on existing systems to exactly formulate such relationships between the parameters.

The red lines in Fig. 4 present the results of the base case LCA model regarding the GHG performance at the study site. At 96.1 gCO_{2eq}/kWh_{th} when considering the current electricity mix, the base case GHG emissions are higher than for a typical ATES system represented by the median value of the MC distribution. This can possibly be explained by the fact that the heat pump at the "Bonner Bogen" ATES system is used for both heating and cooling while the LCA regression model is based on



	Reference	GHG_{ATES} [gCO_{2eq}/kWh_{th}]
a	Schüppler et al. (2019) [3]	54 (mean)
b	Vanhoudt et al. (2011) [48]	79
c	Base case "Bonner Bogen" [this study]	96
d	Tomasetta (2013) [19]	120
e	Moulopoulos (2014) [21]	137

Fig. 5. Comparison of the GHG emission results of the MC simulation using the LCA regression model and GHG emissions of ATES systems described in the literature.

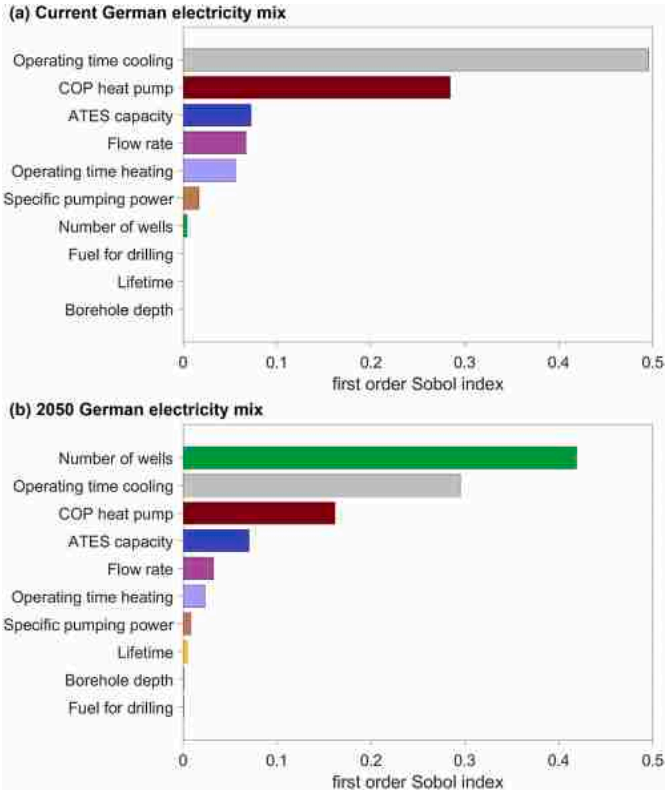


Fig. 6. First order Sobol indices of the ten model input parameters from the LCA regression models using the current German electricity mix (**a**) and the projected 2050 electricity mix (**b**). The top five parameters cause more than 95% of the model output variance.

direct cooling without the need of a heat pump. Furthermore, the system's heat pump operation partially shows low COP values of below 2.5 (Knauber Contracting GmbH, personal communication, May 11, 2018).

Fig. 5 shows a boxplot of the GHG emission results obtained with the MC simulation using the LCA regression model. The upper and lower whiskers indicate the quantiles 97.5% and 2.5%, respectively. Next to the box plot, the figure shows the GHG emissions of specific ATES systems reported in the literature. The comparison reveals that the GHG emission range marked by the whiskers matches the emission values from the literature. This observation verifies the robustness of the regression model and the suitability of the utilized parameters to give reliable estimations for GHG emissions of ATES systems. Thus, the regression model can serve as a simple and fast to use but still robust LCA tool for decision makers.

The ability of the regression models to be easily implemented within a Monte Carlo simulation framework results from their simple linear form (Eq. (1)). The combination of Monte Carlo simulation and regression models offers a time-saving way to gain an overview of GHG emission results from 10,000 different ATES configurations. Obtaining the same number of results using conventional LCA frameworks would be rather time-consuming, particularly the collection of adequate input and output data for creating the LCIs is labour-intensive. Instead, the purpose-built parameterized LCA on which the LCA regression models are based uses variable parameters to adjust the amount of individual LCI items, allowing easy adaptation to other ATES configurations. In addition, the regression models speed up and simplify the applicability for a large number of configurations by alleviating the computational costs of the life-cycle impact assessment. This is shown by the difference in computation time when using the parameterized LCA model in SimaPro and the LCA regression model. The computation time of the parameterized LCA model is about 34 min, while the regression model takes less than a second to complete the generation of 10,000 different ATES configurations and the calculation of their respective GHG emissions. Both computational times refer to the same workstation with 8 CPU cores with a base clock of 3.6 GHz and 128 GB of RAM. It should be noted, however, that the parameterized LCA model in SimaPro calculates other types of environmental impacts in addition to GHG emissions.

3.3. Sensitivity analysis

Fig. 6a shows the first order Sobol indices of the ten parameters included in the LCA regression model (Eq. 2) considering the current German electricity mix determined by GSA. The two parameters with the highest Sobol indices are *operating time cooling* and *COP heat pump*. It is important to emphasize that a Sobol index of around 0.5 does not mean that the respective parameter is mainly responsible for the emission of greenhouse gases, but it has the greatest influence on the variance of GHG emissions per kilowatt hour of thermal energy that is provided by the ATES system. The parameters *ATES capacity*, *flow rate (whole system)* and *operating time heating* also contribute a relevant proportion to the output variance. Together, these five key parameters are responsible for more than 95% of the variance of the GHG results. Thus, when using the regression model for the LCA of a specific ATES system, it is particularly important to use accurate values for these five key parameters in order to obtain reliable results. The findings of the GSA also show which parameters in particular should be optimized when planning new systems.

It is noticeable that the five most influential parameters in Fig. 6a are related to the operation phase of an ATES system. The high Sobol index of the parameter *operating time cooling* is related to its very wide value range (Table 2). An increase in this parameter causes the specific GHG emissions per kilowatt hour of thermal energy to decrease. This is due to the direct cooling without the use of a heat pump as assumed in the present study. The findings therefore confirm that ATES cooling should be done directly whenever possible. The importance of an appropriate design for the heat pump while planning an ATES system is demonstrated by the high influence of the parameter *COP heat pump*. The decreasing demand of electrical power when increasing the heat pump's COP causes lower specific GHG emissions. The LCA regression model confirms this effect. In contrast, the parameters *flow rate* and *operating time heating* have a detrimental effect on the GHG emissions when increased. Regarding the *flow rate*, this can be explained by the additional electrical power needed for a higher volume of produced groundwater. One possibility to reduce the required flow rate is to increase the difference between production and injection temperatures in order to obtain a higher amount of thermal energy per flow rate.

While a higher operating time in the heating mode increases the amount of thermal energy provided by the ATES system, this also leads to a higher amount of electrical energy needed for operating the heat pump. Both effects considered, according to the LCA regression model an increase in the parameter *operating time heating* causes higher specific GHG emissions.

The GSA results of the LCA regression model incorporating the 2050 electricity mix are illustrated in Fig. 6b. The parameter with the highest Sobol index is now *number of wells*. The Sobol indices of the five previously identified most influential parameters in Fig. 6a are accordingly lower. This reflects the decreased importance of the electrical power necessary for ATES operation due to the much lower specific GHG emissions of the projected 2050 electricity mix.

The LCA regression models could now be further simplified by including only the key parameters with high Sobol indices. However, this step is beyond the scope of this study. Due to the very high percentage of variance explainable by the upper five parameters in Fig. 6, only minor deviations in the GHG emissions would be expected from such simplified models.

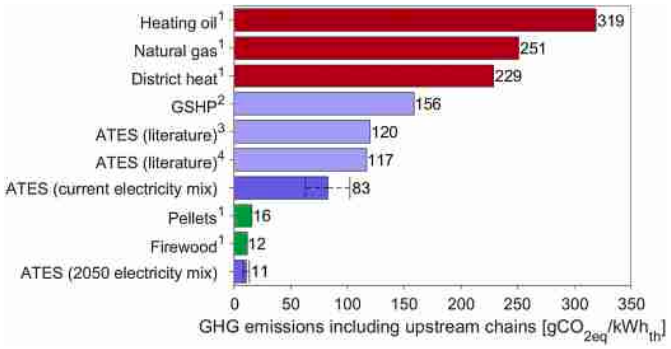


Fig. 7. Specific GHG emissions of different types of heating systems. The two results for ATES determined in this study correspond to the median value of the respective MC results distribution and their interquartile range. [1] [45]; [2] [46]; [3] [19]; [4] [21].

3.4. Greenhouse gas savings

Fig. 7 compares the GHG emissions of different types of ATES and conventional heating systems in order to determine possible GHG savings. The value shown for ATES systems determined in this study corresponds to a typical ATES system, i. e. the median of the MC distribution when using the current German electricity mix (blue dashed line in Fig. 4a). It should be noted that the functional unit of the LCA regression model refers to the combined heating and cooling output of ATES systems, and therefore it does not allow separate assessments of the heating and the cooling phases. Thus, the value of 83.2 gCO_{2eq}/kWh_{th} for the typical ATES system comes from a bimodal system employed for heating and for cooling.

The two types of heating energy that cause the highest GHG emissions are also the ones with the highest shares of the German heating energy mix. Heating oil and natural gas provide around 70% of the heating energy in the German building sector [47]. According to the values in Fig. 7, a typical ATES system can save around 74% of GHG emissions compared to heating oil, and 67% with respect to natural gas. Thus, the use of ATES systems can significantly reduce the GHG emissions in the building sector. The values agree well with the study by Fleuchaus et al. [4], in which the possible savings of ATES systems compared to conventional technologies are between 40% and 70%. The investigations of the ATES of a Belgian hospital by Vanhoudt et al. [48] showed an annual reduction in CO_2 emissons of up to 77% compared to the reference technology comprising of a gas-powered boiler and a compression refrigeration machine.

When comparing the environmental performance of a typical ATES system with wood pellets and firewood, it is important to note that those values also account for the uptake of CO_2 into the biomass. Hence, burning pellets and firewood only releases CO_2 that was previously bound during the plants‘ growth leading to extremely low GHG emissions which are solely caused by upstream processes such as transportation and necessary processing steps [45].

Fig. 7 also shows the LCA results regarding GHG emissions of two specific ATES systems discussed in the literature [19,21]. It is important to note that the environmental impact of the auxiliary gas boiler and the waste water treatment originally included as separate LCA stages in Moulopoulos [21] were disregarded here in order to allow for an appropriate comparison with the other ATES LCAs in Fig. 7. The values of both Moulopoulos [21] and Tomasetta [19] are higher than the GHG emissions of a typical ATES system as determined in this study, even exceeding the upper limit of the interquartile range of this study’s LCA results. Possible explanations for the higher GHG emissions compared to this study’s result are different LCI databases and impact assessment methods. Furthermore, non-ideal operation of the two systems elaborated in the corresponding studies could also cause higher GHG emissions. This is particularly true for the ATES system described by Tomasetta [19], which is only used for heating and thus deviates from the combined operating principle assumed in this study. This deviation illustrates the problematic lack of a precise and universal definition of ATES. In fact, one can argue that the system evaluated by Tomasetta [19] is not even an ATES but merely a groundwater heat pump (GWHP) system.

When using the projected 2050 German electricity mix to operate the ATES systems, the median of the MC distribution (blue dashed line in Fig. 4b) is around 11 gCO_{2eq}/kWh_{th}. This is the lowest value shown in Fig. 7, further demonstrating the outstanding significance of the chosen electricity mix regarding the systems’ GHG performance.

Bonamente and Aquino [46] conducted an LCA of a GSHP system used for heating and cooling. The obtained results show considerably higher GHG emissions compared to the typical ATES system from the present study. It should be noted that the authors provide no information about the electricity mix used to operate the GSHP system. A mix largely consisting of fossil fuels however, is strongly implied. Similar to this study they showed the importance of utilizing electricity resulting from carbon-neutral fuels.

Another evaluation of possible GHG emission savings by GSHP systems was performed by Blum et al. [9] (not shown in Fig. 7) for the southwestern part of Germany. When using the German electricity mix at the time of the study, the resulting GHG emissions of a typical GSHP system are 149 gCO_{2eq}/kWh_{th}. The utilization of a regional mix largely consisting of nuclear and renewable energies reduces the emissions to 65 gCO_{2eq}/kWh_{th}. It should be pointed out however, that the authors did not consider any upstream chain processes or materials and the emissions solely result from the operation of the GSHP systems.

Fig. 7 and the above stated results refer to possible GHG savings when comparing ATES with other types of heating systems. In the case of cooling, the variety of different systems is much smaller, as most of the space cooling demand is currently provided by electricity-driven vapor compression systems [49]. Hence, to be able to estimate possible GHG savings in cooling mode, the median value for ATES systems of 83.2 gCO_{2eq}/kWh_{th} must be compared with the utilized electricity mix and the COP of the cooling system needs to be considered. The most recent numbers from 2019 for the German electricity mix state an emission factor of 401 gCO_2/kWh_{el} [50]. Assuming typical COP values for vapor compression systems ranging between 2 and 4, the possible GHG savings are between 59% and 17%.

The German climate protection policy targets carbon neutrality by 2045 [51]. One pillar of the German energy transition is an increased share of renewable energies in the heating energy mix, which at present is dominated by natural gas and heating oil. Currently, about 70% of the energy for space heating in Germany is provided by these two energy sources [47]. The average energy demand of a German household for space heating and hot water is about 15,600 kWh per year [52]. Assuming that heating oil and natural gas were to be completely replaced by thermal energy supplied by ATES, the average absolute GHG emission savings would amount to about 2100 $kgCO_{2eq}$ per household and year. This amount is equal to a distance of 22,100 km travelled by car, assuming the average fleet emission target value of 95 gCO_2/km that was set by the European Union from 2020 onwards. The high emission savings shown here could be used as an incentive to include ATES in climate protection policies, next to other types of renewable energy supply. An example of a successful energy market penetration of ATES are the Netherlands where market incentive programs and low legislative barriers lead to a high attractiveness of ATES [4].

3.5. Economic comparison

Here, a brief overview of existing economic analyses of ATES is provided, focusing on comprehensively described ATES systems for which information about capital and operational costs are available. This allows the calculation of payback times when comparing ATES to a reference heating and cooling technology. Fig. 8 shows these costs for

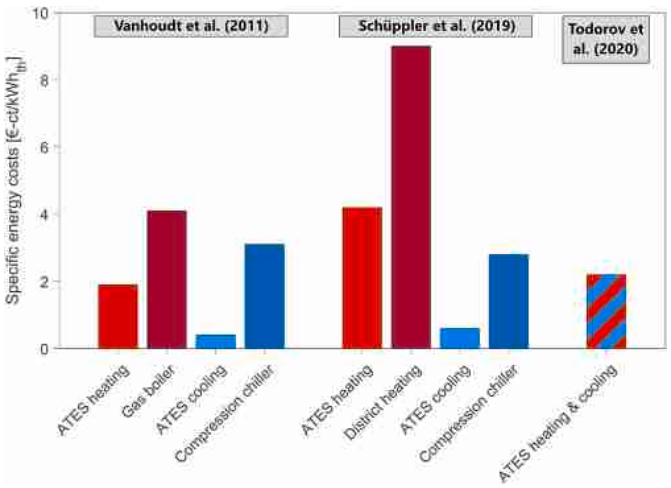


Fig. 8. Specific energy costs of several ATES systems described in the literature compared to the costs of typical conventional heating and cooling systems.

ATES systems and reference technologies that are described in the literature (see also Supplementary data, SD5).

Vanhoudt et al. [48] studied an existing ATES system used for the heating and cooling of a Belgian hospital and performed a cost comparison with a conventional reference system consisting of a compression chiller and a gas-fired boiler. Compared to the reference system, the operational costs of the ATES system are 85% and 55% lower in cooling and in heating mode, respectively. The operational costs are expressed as specific energy costs in €-ct per kWh$_{th}$ of heating or cooling energy that is provided by the considered system. Taking into account the capital costs of the ATES system and the lower operational costs compared to the reference system, a payback time of 8.4 years was determined [48].

Schüppler et al. [3] described an ATES system that was considered to supply a hospital in Germany with heating and cooling energy. Like in the system studied by Vanhoudt et al. [48], the cooling is done directly, while the heat supply is supported by a heat pump. The average specific energy costs were calculated as 4.2 €-ct/kWh$_{th}$ in heating mode and 0.6 €-ct/kWh$_{th}$ for cooling. Thus, they are again significantly lower than the operational costs of the reference system consisting of district heating and cooling using compression chillers (Fig. 8). The calculated average payback time of 2.7 years is significantly lower than for the ATES system described by Vanhoudt et al. [48]. This can be explained by the low heating costs of the gas boiler which was considered as a reference system for the Belgian hospital as well as the relatively high capital costs of the Belgian ATES system. It should also be noted that the payback time in Schüppler et al. [3] does not only result from lower specific energy costs, but also considers the maintenance and replacement costs. The payback time of 2.7 years is in good agreement with the ATES system described by Ghaebi et al. [53], whose payback time related to the reference technology (compression chiller and gas boiler) is about 2.9 years.

The combined specific energy costs for heating and cooling using an ATES system described in Todorov et al. [7] are 2.2 €-ct/kWh$_{th}$, corresponding well to the costs of the other ATES systems in Fig. 8.

The energy cost savings and resulting short payback times of reported ATES systems clearly demonstrate that ATES systems not only help to reduce greenhouse gas emissions but are also an economically viable alternative to conventional heating and cooling technologies. This is further supported by other ATES systems reported in the literature and compiled by Schüppler et al. [3]. The average payback time of the systems used for both heating and cooling is about 6 years. Fleuchaus et al. [4] state that typical payback times of ATES systems reported in the literature range from 2 to 10 years when compared to conventional technologies such as gas or oil boilers and compression chillers.

4. Conclusions

Using a base case LCA of the ATES system at the "Bonner Bogen", an LCA regression model is created including ten relevant system parameters. Due to the parametric structure of the model, it can be applied for the LCA of a wide range of different ATES configurations. Hence, the model is a fast alternative to conventional time-consuming and labour-intensive LCAs. The combination of a Monte Carlo simulation with the LCA regression model enables for the analysis of environmental impacts of a large variety of hypothetical ATES systems and therefore the evaluation of the technology as a whole. Based on our simulations, the median GHG emission of an ATES system is 83 gCO$_{2eq}$/kWh$_{th}$. Compared to conventional heating systems using heating oil and natural gas, 74% and 67% of GHG savings can be achieved, respectively. In comparison to cooling techniques using the current German electricity mix, an ATES system can save up to 59% of GHG emissions. These savings clearly demonstrate that the ATES technology can make an important contribution to more climate-friendly heating and cooling supply in the future. It is also revealed that these GHG savings will significantly increase with the expected growing share of renewable energies in the electricity mix. Thus in the future, GHG savings of up to 97% are achievable when compared to conventional oil heating.

Besides GHG emissions, future research should also be directed towards other environmental impacts. Especially in case of an unbalanced system operation with an elevated heat input into the ground, detrimental effects on the groundwater ecosystem are to be expected that are difficult to investigate with available LCA frameworks.

A brief overview of relevant studies shows that ATES can also offer economic advantages compared to conventional heating and cooling systems. The reported payback times of various ATES systems are significantly lower, ranging between 2 and 10 years. A combined utilization of LCA and a life cycle cost analysis could further quantify CO_2 abatement costs and reveal possible economic advantages of ATES in comparison to other technologies in a more comprehensive way.

Credit author statement

Ruben Stemmle: Writing – original draft, Conceptualization, Methodology, Visualization, Philipp Blum: Supervision, Simon Schüppler: Writing – review & editing, Paul Fleuchaus: Supervision, Investigation, Melissa Limoges: Investigation, Peter Bayer: Writing – review & editing, Kathrin Menberg: Supervision, Conceptualization, Writing – review & editing.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rser.2021.111560.

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