Constrained multi-objective optimization of thermocline packed-bed thermal-energy storage

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HIGHLIGHTS

- Multi-objective optimization of thermal-energy storage.
- Pareto optimal designs.
- Most efficient storage for given cost.
- Cheapest storage for given efficiency.

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ABSTRACT

A constrained multi-objective optimization approach is applied to optimize the exergy efficiency and material costs of thermocline packed-bed thermal-energy storage systems using air as the heat-transfer fluid. The axisymmetric packed-bed's height, top and bottom radii, insulation-layer thicknesses, and particle diameter were chosen as design variables. The competing objectives of maximizing the exergy efficiency and minimizing the material costs were treated by a Pareto front. The Pareto front allows identifying the most efficient design for a given cost or the cheapest design for a given efficiency and is an important tool to find the best overall design of storage systems for a specific application. Constraints were imposed to obtain storage systems with specified capacities and limits on the air outflow temperatures during charging and discharging. The results showed that a storage shaped as a truncated cone with the smallest cross-section at the top has a higher exergy efficiency than storages shaped as cylinders or truncated cones with the largest cross-section at the top. The higher efficiency is attributed to the axial temperature distribution in the packed bed and the associated conduction heat losses across the insulated walls. The optimization of an industrial-scale storage allowed identifying a design with an exergy efficiency that was only 4.8% below that of the most efficient design, but a cost that was 81.3% lower than the cost of the most efficient design. Compared to brute-force design approaches, the optimization procedure can reduce the computational time by 91–99%.

1. Introduction

Thermal-energy storage (TES) systems are required when a time delay exists between the availability of and the demand for thermal energy. TES systems are key components of concentrated solar power (CSP) and advanced adiabatic compressed air energy storage (AA-CAES) plants. For both CSP and AA-CAES plants, the integration of a TES improves the system efficiency and the competitiveness on the electricity market [1,2]. Thermocline TES systems using a packed bed of rocks as sensible storage material are especially suitable because they require only low-cost storage materials and have been shown to have high thermal efficiencies [3].

The development of a thermocline TES system requires that many designs be investigated and evaluated to select a design that is in some sense optimal. Each design can be characterized by a set of operational, geometrical, thermophysical, and performance parameters, see Table 1. The operational parameters are in general defined by the application in CSP or AA-CAES plants, the geometrical parameters are usually arbitrary but need to satisfy structural constraints, the thermophysical parameters depend on the materials used and are usually a function of the temperature and pressure (and therefore the operational parameters), and the performance parameters are used to assess and...
compare designs. The large number of geometric parameters results in a very high-dimensional design space. For example, considering ten values each of the storage height, the top and bottom radii, the thicknesses of two insulation layers, and the particle diameter results in very high-dimensional design space. For example, considering ten variables, such as for multiple structural and insulation layers.

Indicates that several instances of the given parameter exist, such as for multiple structural and insulation layers.

Table 1
Operational, geometrical, thermophysical, and performance parameters of thermocline packed-bed TES systems. The subscript i indicates that several instances of the given parameter exist, such as for multiple structural and insulation layers.

<table>
<thead>
<tr>
<th>Operational parameters</th>
<th>Thermophysical parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flows: mfi, mdi</td>
<td>Thermal conductivities: kji, kbi, kmini</td>
</tr>
<tr>
<td>Charging/discharging times: tci, tdj</td>
<td>Densities: ρfi, ρdi, ρmini</td>
</tr>
<tr>
<td>Inflow temperatures: Tci, Tdi</td>
<td>Heat capacities: cp1, cp2, cpmini</td>
</tr>
<tr>
<td>Charge/discharging pressures: Pci, Pdi</td>
<td>Viscosity: μj</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Geometrical parameters</th>
<th>Performance parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>TES (packed-bed) height: HPB</td>
<td>Outflow temperature changes: ΔTpb, ΔTbd</td>
</tr>
<tr>
<td>Structural thicknesses: lw,i, lb,i</td>
<td>Net discharged energy: Edis</td>
</tr>
<tr>
<td>Insulation thicknesses: lw,i, lb,i</td>
<td>Supplied energy: Es</td>
</tr>
<tr>
<td>Particle diameter: dp</td>
<td>Efficiencies: ηex</td>
</tr>
<tr>
<td>Packed-bed porosity: z</td>
<td>Cost: CTES</td>
</tr>
</tbody>
</table>

Abbreviations
AA-CAES advanced adiabatic compressed air energy storage
CSP concentrated solar power
FG foam glass (insulation)
HTF heat-transfer fluid
LDC low-density concrete
MP microporous (insulation)
SQP sequential quadratic programming
TES thermal-energy storage
UHPC ultra-high-performance concrete
use selected geometrical parameters as design variables and selected performance parameters as objective functions and constraints. Prior studies can be classified into two groups according to whether a single- or multi-objective optimization was performed. Most single-objective optimization studies optimized only the storage efficiency while multi-objective optimization studies optimized both the storage efficiency and cost. First, we review single-objective optimizations. Torab and Beasley [5] appear to have presented the first optimization study of a packed-bed TES by applying a monotonicity optimization method to maximize the heat storage capabilities of the TES. The design variables were the packed-bed height, the particle diameter, and the ratio of packed-bed cross section to particle diameter, while the maximum pressure drop, maximum outflow temperature, and total amount of supplied energy were used as constraints. Their results showed that for a given packed-bed volume, mass flow rate, and charging time, decreasing the particle diameter and increasing the packed-bed height led to increases in the exergy efficiency and decreases in the ratio of the available energy to the total pumping energy. Ammar and Ghoneim [6] used a direct search method to maximize the ratio of the stored energy to the required pumping energy. The packed-bed height, particle diameter, and mass flow rate were used as design variables. Linear constraints were imposed on the design variables and the pressure drop was used as a non-linear constraint. The charging time was chosen such that the outflow temperature reached 95% of the inflow temperature. Their results showed that increasing the particle diameter degrades thermal stratification.

We now turn to reviewing prior work on multi-objective optimizations where the TES efficiency and costs were optimized simultaneously. Maaliou and McCoy [7] predicted the transient temperature profile in a packed-bed TES to calculate the stored thermal energy. The objective of their optimization study was to maximize the difference between the economic value of the stored thermal energy and the capital and operating costs of the TES. The optimum was found with a direct search method using the mass flow rate, TES height, and particle diameter as design variables. The study showed that the height and the particle diameter are limited by increasing pumping costs and that the capital requirements associated with large TES heights counteract the economic value of the stored thermal energy. Choudhary et al. [8] investigated the influence of geometrical and operational parameters of a packed-bed TES system using rocks as storage material coupled to a solar air heater with the goal of maximizing the stored thermal energy at low material costs. The design variables consisted of the charging time, mass flow rate, TES height and cross section, particle diameter, and void fraction. They concluded that the void fraction and the particle diameter have an insignificant influence on the cost and performance of the TES and that the cross section and mass flow rate have to be selected depending on the particular application. Domański and Fellah [9] used a thermoeconomic analysis to minimize the total cost of owning, maintaining, and operating a sensible TES system while maximizing its exergy efficiency. The study investigated the influence of the charging temperature and mass flow rate on the exergy efficiency and showed the trade-off between minimizing the cost and maximizing the efficiency of a TES system. White et al. [10] applied a stochastic optimization algorithm to maximize the exergy efficiency and minimize the investment costs of packed-bed TES for hot and cold storages of a pumped TES system and for an AA-CAES plant. The design variables consisted of the TES height-to-diameter ratio (fixed for the AA-CAES TES), particle diameter, and number of packed-bed segments while the mass of storage material was kept constant. The study showed that a packed-bed segmentation reduces the thermal loss between 25% and 50% and is beneficial to maximize the efficiency and reduce the costs of cold and large-scale TES systems. Cárdenas et al. [11] performed a parametric study to investigate the influence of the TES height-to-diameter ratio, particle diameter, and storage material mass on the exergy efficiency and profitability of an industrial-scale packed-bed TES. Based on a single charging-discharging cycle, the study showed that a small TES height-to-diameter ratio increases the exergy loss due to overcharging and an increase of the storage material mass is beneficial for the exergy efficiency but reduces the profitability.

The work described in the above-mentioned publications suffers from two drawbacks. The first and major drawback is that the physical models used to simulate the performance of packed-bed TES were based on significant simplifications. Therefore, the accuracy of the simulations may be limited and what are claimed to be optimal designs may in fact be non-optimal. Addressing this drawback by using a more sophisticated physical model is the overarching objective of the present work. In contrast to previously used models, our physical model allows for non-cylindrical geometries; temperature-dependent thermophysical properties; multiple structural and insulation layers with different thicknesses; and variable charging, discharging, and idle periods [4]. A second and lesser drawback of the above-mentioned publications is that the optimization methods used to find optimal geometrical and operational parameters were quite simple. This drawback can be tolerated for physical models based on significant simplifications. However, once more sophisticated physical models are used—as in the present work—more sophisticated optimization methods are required to contain computational costs.

Optimization methods can be grouped into two main classes: gradient-free and gradient-based. An extensive review and comparison of gradient-free methods is given in [12]. In general, gradient-free methods use a stochastic approach that can be applied to objective functions that are discontinuous or that have multiple local extrema. However, to have high accuracy, gradient-free methods usually require a large number of evaluations of the objective function [13,14]. This makes gradient-free methods impractical for objective functions whose evaluation is computationally costly. On the other hand, gradient-based methods usually require fewer evaluations of the objective function to find the optimum because the gradient contains additional information about the steepness and extrema of the objective function. The additional information makes gradient-based methods particularly suitable for objective functions that are costly to evaluate [15,16]. In the class of gradient-based methods, the sequential quadratic programming (SQP) algorithm is especially efficient for objective functions subject to linear and non-linear constraints [17]. Apart from these advantages, gradient-based methods have some drawbacks: they do not perform well for discontinuous objective functions, finding global extrema can be difficult for objective functions with local extrema, and determining gradients of the objective function adds complexity to the optimization [18].

We form the objective function from the exergy efficiency at the quasi-steady state and the material costs, subject to constraints on the net discharged energy, packed-bed volume, and outflow temperatures. The objective function is expected to be continuous and to have a single maximum, which suggests that a gradient-based optimization method be used. Furthermore, because reaching the quasi-steady state often requires that a large number of charging-discharging cycles be simulated, the objective function can be relatively expensive to compute. To decrease the computational cost, the number of evaluations of the objective function should therefore be small. For these reasons, the gradient-based SQP algorithm was selected as the optimization method.

The contributions of this work are twofold. First, we present a design method for packed-bed TES systems obtained by coupling the optimization method with a previously developed code for such systems [4]. Second, we apply this design method to several packed-bed TES systems that use rocks as the heat-storage medium and atmospheric air as the heat-transfer fluid (HTF). The design method is described in Section 2 and verified and validated in Section 3. In Section 4, we apply the method to the design of pilot-scale and industrial-scale TES units. A summary and conclusions are presented in Section 5.
2. Design method

The design method is obtained by coupling a previously developed TES code [4] with the optimization package NPSOL [19,20], which provides an implementation of the SQP method.

2.1. TES code

The TES code is based on a one-dimensional thermal non-equilibrium model for packed-bed thermocline storage systems, implemented in Fortran 95. The model includes convective, conductive, and radiative heat-transfer contributions, uses temperature-dependent thermophysical properties, and includes losses through the top, side, and bottom walls of the storage. The model can represent non-cylindrical storage geometries and the walls can consist of multiple structure and insulation layers with variable thicknesses. The temperature fields in the structure and insulation layers are determined in two dimensions to accurately predict thermal losses. The heat-transfer coefficient between the fluid and solid phases is based on the correlation of [21]

\[
Nu = \frac{2.06 \nu}{\varepsilon} Re^{0.425} Pr^{1/3}
\]  

(1)

The pressure drop is calculated using Ergun’s equation [22]

\[
\frac{\Delta P}{L} = \frac{m^* \psi}{\rho_d} \left( C_1 \left( \frac{1 - \varepsilon}{\varepsilon} \right)^2 + \frac{1 - \varepsilon}{\varepsilon^2} \right)
\]  

(2)

where \( \Delta P/L \) is the pressure drop per unit length, \( m^* \) is the mass flux, \( \psi = 0.6 \) is the sphericity of the rocks, and \( C_1 = 217 \) and \( C_2 = 1.83 \) are constants applicable for randomly shaped gravel [23]. Further details of the TES model, in particular on the computation of the temperature fields in the structure and insulation layers and the numerical implementation, can be found in [4].

2.2. Optimization package

The optimization package NPSOL uses the SQP method to minimize an objective function that depends on design variables and linear and non-linear constraints [24]. The optimization problem can be formulated as

\[
\text{minimize } f(\vec{x}) \text{ subject to } \vec{r}(\vec{x}) \leq \vec{u} \text{ with } \vec{r}(\vec{x}) = \begin{bmatrix} \vec{r} & \vec{\xi} \\ \vec{\tau} & \vec{c} \end{bmatrix}(\vec{x})
\]  

(3)

where \( \vec{x} \) is a vector of \( n \) design variables, \( f(\vec{x}) \) is the objective function, \( \vec{r} \) and \( \vec{u} \) are vectors with the lower and upper bounds of each design variable, \( \vec{\xi} \) is a \( m \) \times \( n \) matrix describing the \( m \) linear constraints, and \( \vec{c} \) is a vector with \( m \) non-linear constraint functions. The values of \( \vec{r}, \vec{u}, \vec{\xi}, \vec{c} \), and the initial values of \( \vec{x} \) must be provided as input parameters to NPSOL. The functions \( f(\vec{x}) \) and \( c(\vec{x}) \), the SQP method requires also the gradients of \( f(\vec{x}) \) and \( c(\vec{x}) \) with respect to each design variable.

2.2.1. Complex-step derivative approximation

Gradient-based optimization methods require accurate gradients, i.e., derivatives of the objective function and the constraints with respect to the design variables. A common method to calculate gradients is the finite-difference method. The main problem with the finite-difference method is the so-called step-size dilemma [24]: On the one hand, the step size must be small enough to reduce truncation errors. On the other hand, the step size must be large enough to avoid cancellation errors. To avoid the step-size dilemma of finite-difference methods, the complex-step derivative approximation [25–27] can be used. This approximation uses complex calculus to calculate the derivative without cancellation errors. Therefore, the truncation error can be made very small by reducing the step size and the accuracy of the complex-step derivative approximation can exceed the accuracy of the finite-difference method by several orders of magnitudes [25,27].

The implementation of the complex-step derivative approximation requires that the TES code be “complexified”, which entails (1) converting all floating-point variables and constants in the TES code into complex variables and constants and (2) overloading intrinsic Fortran functions and operators to handle complex arguments. The conversion process is automated by a dedicated code that adjusts all Fortran source files. The overloaded intrinsic functions and operators are collected in a Fortran 95 module similar to [27]. Following the complexification, the derivative of the objective function with respect to the design variable \( x_i \) is approximated as

\[
\frac{df}{dx_i} \approx \text{Im}[f(x_i + ihx_{i+...+x_n})] \frac{1}{h}
\]  

(4)

where \( x_{i+...+n} \) are the design variables and \( h \) is the step size (typically chosen to be \( 10^{-12} \)). The same procedure can be applied to determine the derivatives of any quantity computed by the complexified TES code.

2.2.2. Multi-objective optimization

In general, the objectives in multi-objective optimization are competing, so one objective can be improved only when at least one other objective is worsened [28]. This trade-off can be visualized using the Pareto front, which describes the best possible combinations of the competing objectives [29] and which can therefore be interpreted as the set of solutions that are relevant to making design decisions [15]. The Pareto front can be determined using several methods [30]. One of the simplest is the weighted-sum method, which determines a weighted objective function from

\[
f(\vec{x}) = \sum_{i=1}^{N_h} w_i \hat{f}_i(\vec{x})
\]  

(5)

where \( N_h \) is the number of objectives and \( w_i \) are the weights whose sum is unity. The Pareto front can be computed by varying the weights gradually and computing for each set of weights the optimum of the weighted objective function [15].

In this work, we use the weighted-sum method to combine two objective functions, namely the exergy efficiency of one charging-discharging cycle at the quasi-steady state and the material costs of the TES. The weighted objective function is therefore

\[
f(\vec{x}) = w(1-\eta_{\text{ex}}) + (1-w) \frac{C_{\text{TES}}}{C_{\text{TES,ref}}}
\]  

(6)

where \( \eta_{\text{ex}} \) is the exergy efficiency, \( C_{\text{TES}} \) is the computed material cost of the TES, and \( C_{\text{TES,ref}} \) is an estimated material cost used to normalize \( C_{\text{TES}} \). The normalization is required to obtain a dimensionless cost with a similar order of magnitude to the exergy efficiency. The exergy efficiency is defined by

\[
\eta_{\text{ex}} = \frac{\Xi_{\text{d,ex}} - \Xi_{\text{d,pump}}}{\Xi_{\text{c,net}}}
\]  

(7)

where \( \Xi_{\text{d,ex}} \) and \( \Xi_{\text{d,pump}} \) are the net exergies of the HTF supplied and extracted during charging and discharging, respectively, and \( \Xi_{\text{d,pump}} \) is the thermal exergy required to pump the HTF during a cycle. The net exergy of the HTF extracted during discharging is given by

\[
\Xi_{\text{d,net}} = \Xi_{\text{d,ex}} - \Xi_{\text{d,in}} = \int_0^{\Delta t_d} \left[ m \left( h_f(T_{\text{d,ex}}) - h_f(T_{\text{d,in}}) ight) - T_0 \left( s_f(T_{\text{d,ex}}) - s_f(T_{\text{d,in}}) \right) \right] dt
\]  

(8)

where \( m \) is the mass flow rate of the HTF, \( h_f \) and \( s_f \) are the temperature-dependent enthalpy and entropy of the HTF, respectively, \( T_0 \) is the ambient temperature, and \( \Delta t_d \) is the duration of the discharging phase. An analogous expression holds for \( \Xi_{\text{c,net}} \). The thermal exergy required
for pumping is \[4\]
\[
\Xi_{\text{th,pump}} = \int_{t_{\text{d,in}}}^{t_{\text{d,out}}} \frac{1}{\eta_{\text{Rankine}}E_{\text{tot,sp}}(T_{\text{th,in}})\eta_{\text{pump}}} m \Delta \mu dt
\]
(9)

where \(E_{\text{d,pump}}\) is computed from \[3\]
\[
E_{\text{d,pump}} = \int_{t_{\text{d,in}}}^{t_{\text{d,out}}} \frac{1}{\eta_{\text{Rankine}}E_{\text{tot,sp}}(T_{\text{th,in}})\eta_{\text{pump}}} m \Delta \mu dt
\]
(10)

where \(\eta_{\text{Rankine}}\) is the Rankine cycle efficiency assumed to be equal to 0.35, \(\eta_{\text{pump}}\) is the pump efficiency assumed to be equal to 0.95, \(E_{\text{d,net}}\) is the net extracted thermal energy during discharging given by
\[
E_{\text{d,net}} = E_{\text{d,in}} - E_{\text{d,out}} = \int_{0}^{\Delta t_i} m \left[h_1(T_{\text{th,ina}}) - h_1(T_{\text{th,ina}})\right] dt
\]
(11)

and \(\Delta t_i\) is the duration of the charging phase. In assessing TES designs, it is often instructive to break down the exergetic losses into contributions due to pumping (given by Eq. (9)–(11)), due to thermal losses through the structure and insulation layers, and due to internal heat transfer. The exergetic losses resulting from thermal losses are computed from\(^2\)
\[
\Xi_{\text{th,loss}} = \int_{0}^{\Delta t_i} \left(1 - \frac{T}{T_f}\right) \delta Q_{\text{loss}} dt
\]
(12)

and the exergetic losses due to internal heat transfer follow from
\[
\Xi_{\text{th,HT, int}} = \Xi_{\text{th,net}} - \Xi_{\text{th,pump}} - \Xi_{\text{th,loss}}
\]
(13)

The material cost of the TES is computed from
\[
C_{\text{TES}} = \sum_{i=1}^{N_m} c_i V_i
\]
(14)

where \(N_m\) is the number of materials, \(c_i\) is the volumetric cost of material \(i\), and \(V_i\) is the volume of material \(i\). The material cost includes the storage, structure, and insulation materials. The volumetric costs of the various materials are listed in Table 2. Construction and operation costs are not considered in this work.

2.3. Coupling of TES code with optimization package

A flowchart of the optimization process is shown in Fig. 1. The optimization process depends on the interaction between three components: the TES code, the NPSOL package, and the interface. The purpose of the interface is to handle the data exchange between the TES code and the NPSOL package. Delegating the data exchange to a dedicated interface has two advantages. First, it minimizes the changes required in the TES code and the NPSOL package. Second, it allows the TES code to be executed in parallel since there are usually multiple design variables. The parallel execution is possible because the TES code must be invoked for each design variable and the invocations are independent.

The optimization process starts by generating an input file for the TES code for each design variable. In a given input file, the imaginary part of the respective design variable is set to the step size \(h\) and the imaginary parts of all other design variables are set to zero. For each design variable, the TES code executable is invoked with the respective input file. Once the quasi-steady-state has been reached, the computed objective and non-linear constraint functions are passed to the interface. The interface uses the objective functions \(f(x)\) computed by the TES code and the vector of weights \(w\) to calculate the weighted objective function \(f(x)\) by using Eq. (5). The imaginary parts of the weighted objective and non-linear constraint functions are used to calculate their gradients with respect to each design variable according to Eq. (4). The full set of gradients together with \(\mu, \mu, f(x)\), and \(c(x)\) is passed to NPSOL. The SQP algorithm in NPSOL determines new values of the design variables based on the calculated step length and search direction \[19\]. In a last step, NPSOL checks if the new design variables satisfy the user-specified convergence criteria. If the convergence criteria are satisfied, an optimal set of design variables was found and the optimization process terminates. If the criteria are not satisfied, another optimization iteration is initiated by passing the new design variables to the interface, which adapts the respective input files for the TES code.

In the results presented below, the quasi-steady-state is assumed to have been reached when the relative differences of the real and imaginary parts of the exergy efficiency between two successive charging-discharging cycles are smaller than \(10^{-4}\) and \(10^{-6}\), respectively. Because of the parallel execution of the TES code, the computational time of each optimization iteration is defined by the design variable that requires the most charging-discharging cycles to reach a quasi-steady-state and not the number of design variables.

3. Verification and validation

The verification of the TES model was presented in \[4\]. Several experimental studies were used to validate the TES model, including storages with rocks \[3\] and ceramic particles \[31\] using air as HTF and storages with quartzite and sand using molten salt as HTF \[32\].

The interaction of the TES code and NPSOL was verified using the Rosenbrock function as the objective function in the TES code together with linear and non-linear constraints \[33\]. The minimum of the function found with the optimizer agrees with the analytical minimum subject to the constraints. The agreement demonstrates the proper interaction between the two software packages via the interface and the correct implementation of the complex-step derivative approximation.

4. Results

The results will be presented in three parts. In the first part, the optimization procedure is illustrated using a simple TES configuration characterized by two design variables. This allows the objective and constraint functions to be visualized and to check that the optimizer finds the optimum. In the second part, a pilot-scale TES similar to that considered in \[3\] is optimized for several combinations of design variables. In the third part, the optimization of an industrial-scale TES for a hypothetical CSP plant is presented. For the second and third parts, each multi-objective optimization considers the exergy efficiency and the material costs as objective functions and uses the weighted-sum method to find Pareto-optimal solutions. Each multi-objective optimization uses nine values of the weight \(w = 1.0, 0.99, 0.95, 0.8, 0.5, 0.2, 0.05, 0.01, 0.0\) to form the Pareto front. For all designs, the TES geometry is a truncated cone with variable top and bottom radii. The structure of the TES is given by two concrete layers consisting of ultra-high performance concrete (UHPC) and low-density concrete (LDC), to which are added two layers of microporous (MP) and foam-glass (FG) insulation material as explained in \[3\] and schematically shown in Fig. 2.

To calculate the thermal losses through the structure and insulation

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### Table 2

<table>
<thead>
<tr>
<th>Material</th>
<th>Cost ($/m^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rocks</td>
<td>66</td>
</tr>
<tr>
<td>UHPC</td>
<td>3421</td>
</tr>
<tr>
<td>LDC</td>
<td>737</td>
</tr>
<tr>
<td>MP</td>
<td>4269</td>
</tr>
<tr>
<td>FG</td>
<td>616</td>
</tr>
</tbody>
</table>
layers, the outer wall of the TES is assumed to be at ambient temperature. The thermophysical properties of the structure, insulation, and thermal storage materials and the HTF are temperature-dependent as specified in [34]. The TES is operated such that during charging, the HTF enters the TES from the top and exits from the bottom; during discharging, the flow direction is reversed. To simplify the TES model, the inflow and outflow ports are not directly modeled; instead, the HTF is assumed to enter over the entire cross-section of the packed bed.

4.1. Demonstration of optimization procedure

Consider the design of the pilot-scale TES characterized by the operational and geometric parameters listed in Table 3. The height of the packed bed is fixed at $H_{PB} = 8$ m. The top and bottom radii of the packed bed are used as design variables.

If the TES were designed using the brute-force approach, we would...
choose, e.g., 20 values each for the top and bottom radii, resulting in 400 simulations. Using linear interpolation of the results of these simulations, we could construct contour plots of the exergy efficiency, the material costs, the net discharged energy, and the packed-bed volume as a function of the radii, see Fig. 3. From the contour plots, we could then determine the radii that result in a design with maximum exergy efficiency, for example.

Alternatively, we can design the pilot-scale TES using the optimization procedure presented in Section 2. Fig. 4(a) shows the top and bottom packed-bed radii of each optimization iteration for three initial conditions, superimposed on the interpolated exergy efficiency determined from the 400 brute-force simulations. Fig. 4(b) depicts a close-up of a comparison of the optima computed by the optimization procedure for the three initial conditions, indicated by the symbols, and the optimum determined from the interpolated exergy efficiency, indicated by the dashed lines. As expected, it can be seen that the computed optima coincide with the interpolated optimum and that the computed optima are independent of the initial conditions. Depending on the initial condition, the optimization method requires 12–35 iterations to reach the optimum. Since each iteration requires one simulation of the TES, and the computational time required by NPSOL is negligible relative to that required by the TES code, the optimization reduces the computational time compared to the brute-force approach by about 91–97%. The reduction will become even more significant when the number of design variables is increased.

4.2. Pilot-scale TES

As explained in the introduction and demonstrated in Section 4.1, one advantage of the optimization approach is that compared to the brute-force approach, the computational cost of finding an optimal design is reduced significantly. However, it is not always easy to understand why a particular design is optimal, especially for designs that satisfy several constraints and that are characterized by many design variables. Therefore, with the objective of developing an understanding of the results of the optimization procedure, we consider in this section the optimization of three TES configurations that are subject to the same constraint of $E_{\text{d,net}} \geq 3 \text{ MWh}$ and for which the number of design variables is increased step-wise from two to five. (For all configurations, the computed $E_{\text{d,net}}$ does not exceed 3.3 MWh.) In addition, the first configuration is subject to a second constraint, $V_{\text{PB}} = 300 \text{ m}^3$, see Table 4. Constraints on the HTF outflow temperatures, which are important for practical applications, will be considered in the optimization of the industrial-scale TES presented in Section 4.3. For simplicity, the structure and insulation have the same thicknesses on the top, side, and bottom walls of the TES. The operational parameters are listed in Table 3. The reference material cost $C_{\text{TES,ref}}$ is taken to be $1 \text{ M}$.  

4.2.1. Configuration 1

The first configuration uses $E_{\text{d,net}} \geq 3 \text{ MWh}$ and $V_{\text{PB}} = 300 \text{ m}^3$ as non-linear constraints and the top and bottom packed-bed radii as design variables. Therefore, all Pareto-optimal solutions must lie on the contour line indicating a packed-bed volume of 300 m$^3$ in Fig. 3. Furthermore, because the height of the packed bed is fixed, the TES geometries are conical frustums whose diameter at mid-height is constant.

Fig. 5 depicts the geometries for the designs corresponding to $w = 1.0$ (optimizing for maximum exergy efficiency), $w = 0.0$ (optimizing for minimal material costs), and the intermediate case $w = 0.5$. The geometries are unusual in that they correspond to truncated cones with a non-positive cone angle, i.e., the top packed-bed radius is smaller than or equal to the bottom radius. The reason for the unusual geometry will be discussed below.

The exergy efficiency is shown in Fig. 6 as a function of the top and bottom packed-bed radii. The difference between the radii decreases with decreasing exergy efficiency until a cylindrical shape is reached for the least efficient design. The least and most efficient designs are seen to have exergy efficiencies of just below 92% and just above 95%, respectively.

The material costs of the various designs are presented in Fig. 7. The cost of the storage material is negligible compared to the costs of the structure and insulation materials for all designs. Since the packed-bed volume is constant, the cost of the rocks is constant and cost reductions are therefore achieved by reductions in the volumes of the structure and insulation materials. The cheapest design has a cylindrical shape because this minimizes the surface area per volume and accordingly requires the least structure and insulation materials.

The Pareto front is presented in Fig. 8, which clearly shows the trade-off between maximizing the exergy efficiency and minimizing the material costs. The practical value of the Pareto front is that it allows the identification of the most efficient TES for a given cost and the least expensive TES for a given efficiency. Fig. 8 also presents the exergy-loss breakdown that indicates how the pumping work, thermal losses, and internal heat transfer decrease the exergy efficiency. The definitions of the individual exergy-loss contributions are given in Eqs. (9), (12) and (13). The largest decrease of the exergy efficiency stems from an increase of the thermal losses while the exergy loss due to internal heat
transfer stays almost constant for all designs and the required pumping power is negligible.

Fig. 9(a) shows the net charged and net discharged exergy for each design. The net charged exergy stays constant and with a negligible exergy loss due to the required pumping power, Eq. (7) indicates that the exergy efficiency depends mainly on the net discharged exergy. The net discharged exergy decreases with decreasing air outflow temperature during discharging. The comparison of the HTF outflow temperatures during discharging for designs 1 and 9 is shown in Fig. 9(b). As expected, for both designs the outflow temperature decreases during discharging, but for design 1 the mean outflow temperature is about 11 K higher than for design 9. The higher mean outflow temperature means that the net discharged exergy is higher, leading to an increased exergy efficiency for design 1 compared to design 9.

Fig. 9(b) also shows that during discharging the rate of decrease of the outflow temperature increases considerably for design 1 while for design 9 the decrease is almost linear. This difference can be explained by inspecting the thermoclines of the fully charged and fully discharged states for designs 1 and 9 depicted in Fig. 10. The thermoclines of the two designs differ mainly in the upper section where the hot air enters during charging. Compared to design 9, design 1 has a smaller cross-section in the upper part that leads to a higher velocity of the HTF and accordingly the temperature front moves further down during charging. An additional effect of the higher velocity is a higher Nusselt number that leads to better interphase heat transfer. For these reasons, during the beginning of discharging, the outflow temperature of design 1 is higher than that of design 9.

The optimization predicts that the most efficient designs are shaped like a truncated cone with the smaller cross-section on top and hence have a negative cone angle. This shape is in contrast to existing designs that are either cylindrical [32] or have a positive cone angle [35,36].

The increased efficiency for designs with a negative cone angle results from a reduction of the energy losses through the TES walls, particularly the top wall, and the resulting increase of the mean outflow temperature during discharging. Fig. 11 compares the energy losses for one charging-discharging cycle from the storage material to the structure and insulation materials through the top and side walls. When comparing the cheapest with the most efficient design, the losses through the top and side walls of the cheapest design are about 800%

### Table 4

<table>
<thead>
<tr>
<th>Configuration</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
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<tr>
<td>Performance parameter $E_{\text{dis},\text{net}}$</td>
<td>$\geq 3 \text{ MWh}$</td>
<td>$\geq 3 \text{ MWh}$</td>
<td>$\geq 3 \text{ MWh}$</td>
</tr>
<tr>
<td>Geometrical parameters</td>
<td>$V_{PB}$</td>
<td>$300 \text{ m}^3$</td>
<td>$1 \text{ m}^3$</td>
</tr>
<tr>
<td>$H_{PB}$</td>
<td>8.0 m</td>
<td>0.5–10.0 m</td>
<td>0.5–10.0 m</td>
</tr>
<tr>
<td>$r_{PB,\text{top}}$</td>
<td>0.5–10.0 m</td>
<td>0.5–10.0 m</td>
<td>0.5–10.0 m</td>
</tr>
<tr>
<td>$r_{PB,\text{bottom}}$</td>
<td>0.5–10.0 m</td>
<td>0.5–10.0 m</td>
<td>0.5–10.0 m</td>
</tr>
<tr>
<td>$\bar{v}_{PB}$</td>
<td>0.1 m</td>
<td>0.1 m</td>
<td>0.01–1.0 m</td>
</tr>
<tr>
<td>$d_{PB}$</td>
<td>0.03 m</td>
<td>0.03 m</td>
<td>0.001–0.1 m</td>
</tr>
</tbody>
</table>

Fig. 5. Geometries of Pareto-optimal designs for (a) $w = 1.0$, (b) $w = 0.5$, and (c) $w = 0.0$ of pilot-scale configuration 1.

Fig. 6. Exergy efficiency as a function of the top and bottom packed-bed radii of pilot-scale configuration 1.

Fig. 7. Breakdown of the material costs for the Pareto-optimal designs of pilot-scale configuration 1.

Fig. 8. Exergy efficiency and the exergy-loss breakdown as a function of the material costs of pilot-scale configuration 1.
and 140% larger than those of the most efficient design, respectively. These increases depend mainly on the increased top radius and accordingly the increased surface areas of the top wall and the upper part of the side wall, where the temperatures and the temperature gradients to the outside are higher than in the lower part of the TES. The loss through the bottom wall is negligible compared to the top and side-wall losses because the bottom-wall temperature is close to the ambient temperature. The trend of negative cone angles leading to smaller losses is consistent with the results shown in Fig. 13 of [36].

In prior works, negative cone angles appear not to have been considered because of possible drawbacks related to thermal ratcheting. Thermal ratcheting is a well-known problem in silos and packed-bed TES systems caused by different thermal-expansion rates of the filling and container materials [37,38]. For packed-bed TES systems, different expansion rates can cause the storage material to settle and pack and eventually cause the storage and/or structure materials to fail because of increasing stresses. To prevent material failure, positive cone angles have been suggested to guide the expanding storage material upwards along the inclined wall and hence reduce the stresses on the storage and structural materials [35,36]. In this work, we do not consider mechanical stresses for simplicity. The practical implementation of a packed-bed thermocline storage with negative cone angle may require structured storage materials [39,40] or additional material layers between the storage material and the structure to absorb the mechanical stresses [41].

4.2.2. Configuration 2

The second configuration uses $E_{\text{net}} \geq 3$ MWh as a non-linear constraint and the packed-bed height and the top and bottom radii as design variables. In contrast to configuration 1, the packed-bed volume is therefore not constant. The storage geometries determined by the optimization procedure are depicted in Fig. 12 for $w = \{1.0, 0.5, 0.0\}$. Compared to configuration 1, the storage geometries are seen to be narrower, and, with the exception of the most efficient design, less tall. Fig. 13 shows the exergy efficiency as a function of the (a) packed-bed height, (b) packed-bed volume and (c) material costs. Increasing the height leads to an increased exergy efficiency, but also causes considerable increases in the material costs. The increased exergy efficiency is explained by Fig. 14, which presents the thermoclines at the end of charging and discharging of the most efficient and the cheapest designs. The most efficient design has temperature differences between the fully charged and discharged states of about 5 K and 50 K at the top and bottom of the storage, respectively, whereas the cheapest design has temperature differences of about 190 K and 230 K at the top and bottom of the storage, respectively. Depending on the application of the TES, the minimum and maximum outflow temperatures during the charging-discharging cycle are important operational parameters that need to be considered during the design phase of the TES as explained in Section 4.3. For brevity, the breakdown of the TES material costs is not shown.
4.2.3. Configuration 3

The third configuration of the multi-objective TES optimization uses $E_{\text{net}} \geq 3 \text{ MWh}$ as a non-linear constraint and the packed-bed height, the top and bottom radii, the thickness of the outer insulation layer, and the particle diameter as design variables. The TES geometries for $w = [1.0, 0.5, 0.0]$ are depicted in Fig. 15. Compared to configuration 2, the main difference between the TES geometries is the increased outer insulation-layer thickness of design 1.

Fig. 16(a) shows the exergy efficiency as a function of the outer insulation-layer thickness consisting of foam glass. As expected, the more efficient designs have a larger insulation-layer thickness, which reaches the upper and lower limits of 1.0 m and 0.01 m for the most efficient and for the cheapest designs, respectively. Increasing the insulation-layer thickness reduces the thermal losses through the walls but also increases the material costs as indicated in Fig. 16(b). A breakdown of the material costs is shown in Fig. 17. For all designs, the cost of the insulation materials is the largest contributor to the total costs and the cost of the storage material is negligible. Reducing the required amount of the insulation material is therefore essential to reducing the material costs.

Fig. 18 presents the exergy efficiency and the exergy-loss breakdown as a function of the particle diameter. The exergy efficiency increases with increasing particle diameter. The least efficient design has a particle diameter that is equal to the lower limit of 1.0 mm while the most efficient design has a particle diameter of 21.5 mm and is therefore below the upper limit of 100.0 mm. A decreasing particle diameter influences the TES performance in two ways: it enhances the heat transfer between the solid and fluid phases and it increases the pressure drop over the packed bed. Enhanced heat transfer increases the exergy efficiency while an increased pressure drop drives up the pumping power and therefore decreases the exergy efficiency. The rapid increase of the pumping power for very small particles can be seen from the exergy-loss breakdown in Fig. 18. For design 9, the required pumping power is about 140 times larger than that for design 1.

4.3. Industrial-scale TES

Finally, the optimization procedure is used to optimize an industrial-scale TES for a hypothetical 26 MWel CSP plant [3]. With the exception of the insulation layers, the optimization is based on the same design variables as configuration 3 of the pilot-scale TES. The insulation layers of the industrial-scale TES are characterized by six design variables that allow the thicknesses of the top, side, and bottom walls of the two layers to be varied. The optimization of the industrial-scale TES imposes the non-linear constraints that the air outflow temperatures during charging and discharging be smaller than 393.15 K and greater than 723.15 K, respectively. This corresponds to maximum outflow temperature changes of 100.0 K. The operational, geometrical, and performance parameters are listed in Table 5. The reference material cost $C_{\text{TES,ref}}$ is taken to be $7 \text{ M}$.

Fig. 19 depicts the geometries of the Pareto-optimal designs for $w = (1.0, 0.5, 0.0)$. Similar to the pilot-scale TES results, the most efficient design has a negative cone angle and the cheapest design is cylindrical. In contrast to the pilot-scale results, however, the design for $w = 0.5$ has a small positive cone angle. The transition from the most
The Pareto front and the exergy-loss breakdown are presented in Fig. 20. According to the figure, the best compromise between high efficiency and low costs appears to be design 5 with an efficiency of 94.1%—only 4.8% below that of the most efficient design—at a cost that is 81.3% lower than the cost of the most efficient design. The considerable difference in costs is caused mostly by the large amount of microporous insulation used in design 1. This can be seen from the material-cost breakdown in Fig. 21, which indicates that the microporous insulation accounts for about 75% of the total costs of design 1. For design 2, the concrete and insulation contribute about equally to the total costs while for designs 3 to 9, the major contribution comes from the concrete. As for the pilot-scale TES, the storage material has but a small influence on the total costs.

The large contribution by the insulation to the cost of design 1 is explained by an increased thickness of the insulation layers. This can be seen from Fig. 22, which shows the insulation thicknesses on the top, side, and bottom wall of the Pareto-optimal designs. Design 1, for which the material costs are not included in the objective function, uses the maximum allowed thicknesses for both insulation layers. Designs 6–9, the four cheapest designs, reduce costs by reducing both insulation layers to the minimum. Designs 2–5 use the minimum amount of the expensive microporous insulation, but increase the thickness of the cheaper foam-glass insulation on the top and side walls where the packed-bed temperature is higher. These results show clearly the trade-off between increasing the exergy efficiency by reducing the heat-transfer losses and decreasing the material costs by reducing the amount of expensive insulation material.

Fig. 23 depicts the exergy efficiency as a function of the packed-bed height, the top and bottom packed-bed radii, and the particle diameter for the Pareto-optimal designs. Interestingly, the transition from the most efficient to the cheapest design in terms of the packed-bed height and the particle diameter is not monotonic. For example, the packed-bed heights of the most efficient and cheapest designs are 30.0 m (the upper limit) and 15.5 m, respectively, but design 4 reaches a minimum...
height of 8.2 m. The existence of a minimum height is in contrast to the pilot-scale configurations 2 and 3 for which the heights exhibit a monotonic decrease from the most efficient to the cheapest design. Furthermore, Fig. 23 demonstrates that the top and bottom packed-bed radii decrease from the most efficient to the cheapest design in such a way that the cone angle is negative for design 1, positive for design 2, and almost zero for designs 3–9. The transition from a negative to a positive and back to a neutral cone angle is again in contrast to the monotonically increasing cone angle of the pilot-scale configurations. Finally, Fig. 23(c) shows that the particle diameters for the most efficient and the cheapest designs are 49.5 mm and 10.0 mm, respectively. As for the packed-bed height, however, the trend is not monotonic: design 3 is characterized by a local minimum diameter of 25.5 mm whereas design 5 is characterized by a local maximum diameter of 27.7 mm. The locations of the local extrema of the particle diameter coincide with the change from a decreasing to an increasing packed-bed height. This change in the trends of the packed-bed height and the particle diameter is at least partially explained by the minimum air outflow temperature during discharging, which reaches its non-linear constraint for designs 5–9 as indicated in Fig. 24(b). To avoid falling below the constraint, the optimizer increases the packed-bed height and decreases the particle size for designs 5–9. It should be noted that Fig. 24(a) shows that the constraint on the maximum air outflow temperature during charging is not reached by any of the designs.

Table 5

Operational, geometrical, and performance parameters of the industrial-scale TES.

<table>
<thead>
<tr>
<th>Operational parameters</th>
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<tr>
<td>Mass flow charging/discharging: $m_{\text{air},c}, m_{\text{air},d}$</td>
<td>132.0 kg/s</td>
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<td>Charging/discharging time: $\Delta t_c, \Delta t_d$</td>
<td>8.0 h</td>
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<tr>
<td>Inflow temperature charging: $T_{\text{in},c}$</td>
<td>823.15 K</td>
</tr>
<tr>
<td>Inflow temperature discharging: $T_{\text{in},d}$</td>
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<td>Ambient temperature: $T_0$</td>
<td>293.15 K</td>
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<table>
<thead>
<tr>
<th>Geometrical parameters</th>
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<tr>
<td>Packed-bed height: $H_{\text{PB}}$</td>
<td>5.0–30.0 m</td>
</tr>
<tr>
<td>Top/bottom radius: $r_{\text{t,b},\text{PB}}$</td>
<td>5.0–30.0 m</td>
</tr>
<tr>
<td>1st structure thickness: $l_{\text{UHPC}}$</td>
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</tr>
<tr>
<td>2nd structure thickness: $l_{\text{LDC}}$</td>
<td>0.5 m</td>
</tr>
<tr>
<td>1st insulation thickness: $l_{\text{MP}}$</td>
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</tr>
<tr>
<td>2nd insulation thickness: $l_{\text{FG}}$</td>
<td>0.01–0.1 m</td>
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<tr>
<td>Particle diameter: $d_p$</td>
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<table>
<thead>
<tr>
<th>Performance parameters</th>
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</thead>
<tbody>
<tr>
<td>Outflow temperature change: $\Delta T, \Delta T_0$</td>
<td>100.0 K</td>
</tr>
</tbody>
</table>

Fig. 18. Exergy efficiency and exergy-loss breakdown as a function of the particle diameter for the Pareto-optimal designs of the industrial-scale configuration.

Fig. 19. Visualization of Pareto-optimal designs with (a) $w = 1.0$, (b) $w = 0.5$, and (c) $w = 0.0$ for the industrial-scale configuration.

Fig. 20. Pareto front of the industrial-scale TES optimization together with the exergy-loss breakdown.

Fig. 21. Breakdown of the TES material costs for the Pareto-optimal designs of the industrial-scale configuration. Note the break in the abscissa.
Exergy efficiency is also improved by reducing the pressure drop, which can be achieved by increasing the packed-bed radius and the particle diameter, as for the more efficient Pareto-optimal designs shown in Fig. 23. Conversely, the figure shows that for the less efficient and cheaper Pareto-optimal designs, the packed-bed radius and the particle size decrease and accordingly the pressure drop increases. The increasing pressure drop cannot only be tolerated, but actually becomes advantageous because it is caused by the increase of the flow velocity (resulting from the decreased packed-bed radius) and the decrease of the particle size, both of which improve the internal heat transfer between the solid and fluid phases. The improved internal heat transfer means that the TES volume can be reduced and accordingly the material costs decrease.

Fig. 22. Inner (microporous) and outer (foam-glass) insulation layer thicknesses on the (a) top, (b) side, and (c) bottom walls of the Pareto-optimal designs of the industrial-scale configuration.

Fig. 23. Exergy efficiency as a function of the (a) packed-bed height, (b) top and bottom packed-bed radii, and (c) particle diameter for the Pareto-optimal designs of the industrial-scale configuration.
The optimization of the industrial-scale storage demonstrated the potential of the optimization procedure to significantly reduce material costs while retaining high exergy efficiencies. One design had an exergy efficiency that was only 4.8% below that of the most efficient design, but a cost that was 81.3% lower than the cost of the most efficient design. By using constraints on the changes in the air outflow temperatures during charging and discharging, the procedure can be used to design a TES for specific CSP or AA-CAES plants, for which these temperatures are important parameters for the integration of the TES into the plants.

For the design of TES systems, the optimization procedure presented here is a significant advance over prior optimization procedures. To the authors’ knowledge, this is the first study that investigates the optimization of the packed-bed height, the top and bottom packed-bed radii, the thicknesses of two insulation layers on the top, side, and bottom walls, and the particle diameter of a TES. The procedure can be adapted easily to consider additional design variables, objective functions, and non-linear constraints.

In further work, the non-monotonic behavior of the results for the industrial-scale storage will be investigated and the objective function will be extended to include the construction costs.

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