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Metaheuristic Design Optimization of the Air-PCM Thermal Storage Unit for Solar Air Systems

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Phase change materials (PCMs) and thermal energy storage (TES) represent a way toward sustainable utilization of renewable energy resources. An air-PCM thermal storage unit integrated in solar systems is a device, which employs the latent heat TES to balance between the demand and supply of heat (or cold) for space heating (or cooling) in buildings. Previously published studies demonstrate that this approach is viable but design parameters of the unit need to be optimized. In the paper, a computer model of the heat storage unit was developed and coupled to metaheuristic nature-inspired optimization algorithms with the aim of design optimization of the TES unit. The unit consisted of flat plates made of a PCM, which was macro-encapsulated in aluminium containers. The energy balance and control volume methods were used to build the model and the effective heat capacity technique was applied for phase change modelling. The model was created in Python, validated against experimental data and an open-source optimization library DEAP with metaheuristics was used as an optimization solver. A design optimization problem was specified with including the arrangement of the PCM plates and their thickness. Results showed that the DEAP library and metaheuristics are well applicable for the solution of this kind of optimization problem.

1. Introduction

In recent years, there is an increasing effort of the society toward the utilization of renewable energy resources as a way for minimization of fossil fuel consumption and greenhouse gas production. Currently, a considerable amount of energy is used in the form of heat, especially in buildings and households for space heating. It is well reported that buildings account for about 40 % of the overall energy consumption, see e.g. the review presented by Li et al. (2019). As for increasing the share of renewable energy resources and their utilization to buildings, solar energy seems to be a good candidate as the conversion of solar energy into heat is easy and technically as well as technologically inexpensive. However, a crucial issue related to solar energy is that very often there is a mismatch between energy supply and demand. In other words, the Sun providing solar energy is available during the day but in many cases Sun's solar energy would be much appreciated in the late afternoon, evening, or at night when the demand for space heating arises.

One of promising approaches coping with the mismatch between heat supply and demand is thermal energy storage. The main idea is rather simple: the use of a suitable media allowing for heat accumulation and storage. Once there is a demand, heat is released. Even though sensible heat storage materials such as pebbles can be employed, latent heat thermal energy storage (LHTES) turns out to be more efficient. The LHTES utilizes a material, which undergoes the phase. Since the latent heat of phase change is significantly higher than the sensible heat in the same temperature interval, a relatively high thermal capacity in a narrow temperature range can be achieved. The materials for LHTES are commonly referred to as phase change materials (PCMs) and there is a wide range of PCMs commercially available at the market for various applications with different temperature ranges. Organic PCMs such as paraffin as well as inorganic PCMs such as salt hydrates are typical

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materials used in building applications. Zhou et al. (2012) thoroughly reviewed suitable PCMs for LHTES in buildings. They emphasised that a PCM should have the phase change temperature between 18 °C and 30 °C, should be chemically stable and compatible with encapsulation and other construction materials.

The range of LHTES applications in buildings is rather wide, ranging from integration of PCMs into walls, ceilings, or floors to domestic water heating to the use of storage units and heat exchangers for space heating. Even though many applications of LHTES are related to small-scale applications, there are also examples of large-scale and industrial applications. Guelpa and Verda (2019) reviewed the use of LHTES in district heating and cooling systems and reported that the storage density in such cases is within the range of 40-150 kWh/m^3 with the cost 50-500 EUR/m^3. Royo et al. (2019) reported on the LHTES in high temperature waste heat recovery of industrial furnaces used in energy-intensive industries. Jacob et al. (2019) studied the utilization of solar energy with LHTES for the reduction of natural gas consumption in industrial applications with high temperatures. In the paper, a heat storage unit containing a PCM in the form of thin plates (Compact Storage Modules - CSMs) is considered, which is proposed for operation with a solar air collector as in Charvát et al. (2014). Such configuration allows for the utilization of renewables in buildings: solar energy is transformed into heat with the solar air collector and the PCM integrated into the storage unit enables storing heat for a period of time and releasing it when needed.

Recently, a number of research works have been published on the topic of heat storage units with LHTES. Zhang et al. (2020) investigated the improvement of heat discharging from a LHTES unit using tree-shaped fins. The use of the tree-shaped fins allowed for significant improvement. Rezaei et al. (2020) studied the LHTES unit for high temperatures. In the parametric study, 75 design configurations were evaluated and consequently used in optimization solved using the desirability method. The Pareto frontier was determined by the genetic algorithm. Pu et al. (2020) analysed the radial LHTES unit enhanced with fins and performed the thermal performance optimization. Though several parameters were involved in their study, the authors evaluated a set of scenarios with various values of the parameters rather than using an optimization algorithm seeking for the optimal solution. Sun et al. (2020a) investigated the heat charging process of LHTES unit integrating a PCM in the form of plates. The Taguchi optimization approach was used to determine optimal parameters and a 23 % improvement of the energy charging rate was reported.

The thermal performance of the unit is strongly dependent on its configuration as well as on the weather and climatic conditions where the unit is operated. This means that the configuration of the unit needs to be optimized and an optimum design should be determined to take into account specific local conditions and expected outcomes. In many research papers, the unit and its configuration are proposed according to the experience of engineers, e.g. in (Nada et al. 2019) who experimentally investigated a heat storage unit with PCM plates for free cooling at low temperature differences between the PCM and ambient air. The authors reported that free cooling under low temperature differences is feasible providing certain precautions. In some works, case studies are investigated and the best one is considered as optimal, e.g. in (Sun et al., 2020b). Only a rather limited number of papers deal with optimization in the right sense where an algorithm seeking maximum or minimum of an objective function is used such as by Pu et al. (2020) mentioned above. In this paper, a framework for a true optimization approach is presented and the use and applicability of soft computing methods – metaheuristics – is demonstrated and discussed. A previously created and validated quasi-2D model of the heat storage unit integrating thin plates made of a PCM is employed and coupled with an optimization library. Since the transient model contains a large number of equations related to heat transfer and temperature distribution and their direct integration into the optimization model would result in a large-scale and difficult-to-solve problem, the model of the unit is used in a black-box approach. Python is adopted as a programming interface for both the model as well as for metaheuristic optimization using the DEAP library. Though a simple design optimization problem is considered, the results indicate that the proposed combination of the tools seems effective and applicable for design optimization of the heat storage unit.

2. Air-PCM heat storage unit

The considered heat storage unit is made from a plywood shell in which commercially available thin plates, so-called Compact Storage Modules (CSM), are arranged. The CSM consists of an aluminium container, which is filled with the PCM. Figure 1 shows a photograph and schematic of the unit built for experimental investigation and, in particular, for validation of the computer model described and discussed in the following section. As can be seen in Figure 1, the CSMs are positioned horizontally in five columns with 20 CSMs per each column, which makes 100 CSMs accommodated in the unit. The vertical air gaps of 20 mm between the CSMs allow the air flowing through the unit and exchange heat with the PCM inside the CSMs. The CSMs filled with the paraffin-based PCM RT42 having the mean phase change temperature of 42 °C were installed in the unit (Rubitherm, 2013). The overall thermal capacity of the unit in the temperature range from 25 °C to 55 °C was about 3.3 kWh.

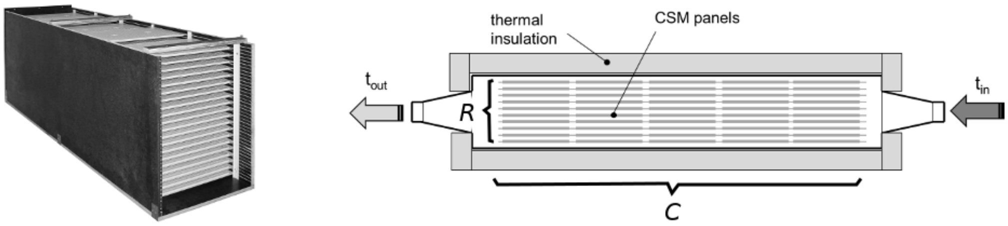

Figure 1: The photograph and schematic of the heat storage unit considered in the paper

The unit was previously studied by the authors computationally as well as experimentally, and the readers interested in details are referred to the research work by (Charvát et al. 2014).

During the daytime when solar radiation is available, the solar air collector is used to convert the solar energy into heat, which is transferred to the air flowing through the collector. The warm air is then fed to the heat storage unit where it flows in the air gaps between the CSMs. If the temperature of the PCM is lower than that of the air, then heat transfer occurs from the air to the PCM meaning that the unit is being charged (heat storage period). As a result, the PCM increases its temperature, undergoes the phase change and melts. Once the heat demand appears (typically in the evening or at night), the cold outdoor air is fed to the unit for its discharging (heat release period). Since the outdoor air has a lower temperature than the PCM, heat transfer occurs from the PCM to the air. As a result, the PCM decreases its temperature and solidifies while the air is heated up. The heated air is then transferred to the room where it is used for space heating.

3. Computer model of air-PCM heat storage unit

The developed computer model of the heat storage unit is a heat transfer model, which solves the temperature distribution of the PCM inside the CSMs as well as the temperature distribution of air flowing in the air gaps between the CSMs. Originally, the model was developed as a type (library) for the simulation system TRNSYS, written in C++ as a standalone model for MATLAB, see the previous works by Charvát et al. (2019) who computationally and experimentally investigated the applicability of the unit for free heating and cooling. In this paper, the model was reimplemented and coupled with the DEAP library of evolutionary optimization algorithms in Python. The model is quasi-2D, which means that a system of independent 1D submodels solves one-dimensional heat transfer in the PCM at various locations along the airflow. The only simulated dimension is in the direction of the thickness of the CSM (perpendicular to the air flowing along the CSMs). Each 1D submodel of the PCM thermally interacts with the air flowing in the air gaps through the unit. The submodels solve the following heat transfer governing equation with phase change:

$$\rho c_{\mathrm{eff}} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \tag{1}$$

where ρ is the density, c_{eff} is the effective heat capacity used for modelling of the phase change, T is the temperature, t is time, k denotes the thermal conductivity, and x is the spatial coordinate, i.e. the location in the PCM. In the model, the bell-shaped effective heat capacity was used. As for the air flowing in the air gaps between the CSMs, the air temperature is determined from the heat balance of between the air and the PCM. The equation used for the determination of the air temperature $T_{\mathrm{air},j}$ in the j-th section of the air gap is:

$$T_{\mathrm{air},j} = T_{\mathrm{air},j-1} - \frac{Q_{\mathrm{loss},j-1} + Q_{\mathrm{PCM},j-1}}{\dot{m}_{\mathrm{air}} c_p \Delta t} \tag{2}$$

where $Q_{\mathrm{loss},j-1}$ is the heat loss from the $(j-1)$-th section, $Q_{\mathrm{PCM},j-1}$ is the heat transferred to or from the PCM, $\dot{m}_{\mathrm{air}}$ is the mass flow rate of the air, c_p is the heat capacity of air at constant pressure, and Δt is the time discretization step. The developed model was investigated, tested, and validated against experimental data in the previous research works of the authors. The readers interested in further details about the development of the model, implementation details, the selection of the effective heat capacity function, the spatial discretization of the air gaps and CSMs with the PCM as well as in the experimental comparison and validation are referred to Stritih et al. (2018).

4. Metaheuristics and optimization library DEAP

Metaheuristic algorithms, or just metaheuristics, are optimization algorithms, which are used especially in cases where traditional optimization methods fail or are computationally expensive and considerably time-consuming.

The metaheuristics do not, in contrast to common mathematical optimization techniques, search for a global and exact optimum as they rather seek a sufficiently good and approximate local optimum. Metaheuristics assert stochastic behaviour, which means that the repeated optimization process does not necessarily give an identical solution. Most of the metaheuristics are inspired by nature and by the behaviour of various animals or species. As an example, the genetic algorithm is based on principles of selection, reproduction, crossover, and mutation over the generations in the evolution of a species. Another example is a firefly algorithm, which is inspired by the behaviour of fireflies in the nature. Individual fireflies move somehow randomly but they also attract each other according to their light intensity. The swarm of fireflies moves as a bulk following the brightest individuals. A detailed description of metaheuristics and functionality/principle of various algorithms can be found elsewhere, e.g. in the textbook by Yang (2010).

As mentioned above, the metaheuristics are effective especially in cases where the traditional optimization methods, widely based on the evaluation of gradients, are inefficient or even fail (Jahangiri et al., 2020). This is often the case of heat transfer problems, which involve computer models. The bottleneck of problems solved with conventional gradient-based algorithms such as the conjugate gradient, steepest descent and the augmented Lagrange multiplier methods (Ruszczynski, 2011) is that the mathematical description of the involved processes contains a (very) a large number of unknown variables, which need to be determined in the optimization process (are typically included in equality constraints). Unfortunately, in many cases, the model describing a process and/or the number of unknowns involved in the model can be much higher than the number of unknowns directly related to the objective (e.g. to a few design parameters). In terms of transient heat transfer solved numerically, all the temperatures in spatial and time nodes represent such phenomena-related unknowns. In particular, the spatial and time discretization of the CSMs with the PCM accommodated in the heat storage unit leads to 3.6×10^{8} unknown variables, assuming 100 CSMs, 100 spatial nodes per each CSM, and 36,000 time nodes for a 10 h simulation with the time step of 1 s. Such the number of variables makes the problem very difficult to solve for methods employing the traditional mathematical programming and optimization. However, in case of metaheuristics, the model is considered as a black-box, which means that the algorithm only needs the evaluation (determination of the value of the objective function) of the model for a certain set of input parameters. In other words, a black-box approach handles the phenomena-related unknowns (temperatures) in a straightforward way without a need to seek them in the optimization process as these unknowns are computed (evaluated) directly from the numerical heat transfer model. Even though such computation of the model has to be performed repeatedly in the loop for various sets of parameters, the overall computational cost is usually considerably lower than in case of the traditional optimization. The approach based on metaheuristics has been already successfully applied in similar engineering problems, see e.g. (Baniasadi et al., 2020) dealing with particle swarm optimization of thermal energy storage systems in smart buildings or (Borunda et al., 2019) applying a genetic algorithm in design of solar collector.

In the paper, the DEAP library in Python was utilized (Fortin et al., 2012). The use of such libraries is highly recommended and preferred over the implementation of the fundamental methods by the user as codes involved in the libraries are well tested, tuned, and optimized for their performance. In contrast to other similar libraries and packages, the user of the DEAP package is not limited to predefined types and methods but he or she can also easily create new ones, which can be adapted to specific requirements. The DEAP library fully employs the object-oriented programming and is based on the use of two modules: creator and toolbox. The creator serves as a constructor allowing the creation of new classes with inheritance. The toolbox is then a package, which includes all necessary attributes, functions, and data containers, which can be used to specify and build the functionality of the algorithm according to the needs of the user.

5. Design optimization of the heat storage unit using metaheuristics

The model of the heat storage unit written in Python was coupled with the DEAP library to assess the optimization capabilities and optimize the design of the unit. The following charging scenario was considered, adopting some simplifying assumptions (Kesler, 2019). The goal (objective function) was to determine the arrangement and thickness of the CSMs in the unit, which would lead to the maximum amount of heat stored in the unit (efficiency of charging). It was assumed that about 62 kg of the PCM RT42 is available, which correspond to 100 CSMs with the RT42 having the thickness of 10 mm. The initial PCM temperature was set to 25 °C and the charging of the unit, which lasted 4 hours, was accomplished with the airflow rate of 230 m^3/h and heated the solar air collector to the temperature of 58 °C. Such parameters correspond to the setup investigated in the previous work of the authors (Charvát et al., 2014).

The arrangement of the CSMs can be described by the pair (C, R) of integers (indicated in Figure 1), one for the number of columns of the CSMs while the other for the number of the CSMs (rows) in each column. Since the plates with the PCM RT42 are commercially available in three thicknesses d of 10 mm, 15 mm, and 20 mm, these values were considered in the study as well. Considering 62 kg of the PCM available, it means that in case of the CSMs with d = 10 mm there were 100 CSMs available for the use in the unit, in case of d = 15 mm there were only 66 CSMs, and in case of d = 20 mm the maximum number of CSMs was 50. In order to avoid excessive and rather impractical dimensions of the unit (e.g. placing all the CSMs into one column), the minimal number of the CSMs per row as well as per column was set to three. As can be deduced from the above description, the configuration of the CSMs in the unit can be described by three integers as (C, R, d). The optimization problem maximizing the heat storage capacity *Q* can be then formulated as follows:

maximise $Q(C, R, d) = \dot{m}_{air} c_{p,air} (t_{air,in} - t_{air,out})$ (3)

subject to $d \in \{10, 15, 20\}$ mm (4)

$C \cdot R \leq N$ where $N = 100$ for $d = 10$ mm (5)

$N = 66$ for $d = 15$ mm (6)

$N = 50$ for $d = 20$ mm (7)

$C, R \geq 3$ and $C, R \in \mathbb{N}$ (8)

where $\dot{m}_{air}$ is the air mass flow rate through the unit, $c_{p,air}$ is the heat capacity of air, $t_{air,in}$ and $t_{air,out}$ is the air temperature at the inlet and outlet of the unit. The parameters to be optimized are C, R, d, while the temperature distribution of the PCM inside the panels corresponding to particular values of C, R, d is determined from the black-box heat transfer model of the unit. The problem described by Eqs(3) - (8) was solved with the use of the DEAP library and two distinct evolutionary algorithms were applied: the particle swarm optimization (PSO) and the genetic algorithm (GA). Each algorithm was launched two times to assess whether the optimal configuration, the heat storage capacity, and the computational time are the same (similar) or not. Table 1 summarizes the results of the optimization processes.

Table 1: Results for the optimal design of the heat storage unit

Parameter	Particle swarm optimisation (PSO)		Genetic algorithm (GA)	
	First run	Second run	First run	Second run
Optimal number of columns (*C*)	20	25	25	25
Optimal number of rows (*R*)	5	4	4	4
Optimal thickness of CSMs (d)	10	10	10	10
Thermal storage capacity	2.8704 kWh	2.8705 kWh	2.8705 kWh	2.8705 kWh
Computing time	4 h 37 min	8 h 5 min	7 h 58 min	7 h 32 min

As can be seen from Table 1, the maximization of the heat storage capacity requires positioning the CSMs in a larger number of columns with only a few CSMs in each column. The optimal configuration with the maximal value of Q is (C, R) = (25, 4) even though the configuration of (C, R) = (20, 5) led to a very similar heat storage capacity. Since the considered problem is relatively simple, "validation" of results can be made by a physical (heat transfer) consideration as follows. The configurations in Table 1 have long air gaps between the CSMs, which allow for maximum heat transfer in terms of the air temperature difference at the inlet and outlet Eq(3). In all cases, the optimal thickness of the CSMs was 10 mm, which is also in agreement with expectations since in this case, the heat transfer area of CSMs is maximal. The thicker CSMs are less efficient due to low thermal conductivity of the PCM. In other words, the thicker the CSM the greater the period of time needed to penetrate, transfer the heat and charge the PCM inside the CSM at its middle plane.

6. Conclusions

The applicability of metaheuristic optimization algorithms to the solution of a problem with thermal energy storage and phase change material (PCM) was investigated. Design optimization of an air-PCM heat storage unit, which can employ solar energy for space heating, was considered. A quasi-2D computer model of the unit was implemented in Python and coupled with the Distributed Evolutionary Algorithms in Python (DEAP) library. Since the model of the unit involved the solution of heat transfer problem and contained a large number of unknown variables, the DEAP library used the computer model of the unit as a black-box. A problem including the arrangement of the PCM plates and their thickness was formulated and the particle swarm optimization and the genetic algorithm were applied. Both the methods provided similar behaviour and found the same optimal solution. The results indicate that the use of metaheuristics and DEAP library seems to be well applicable to the solution of such problems.

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