Design of Experiments applied to numerical simulations: the study case of a PCM-air heat exchanger for temperature maintenance in rooms

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Abstract. This paper studies the design and integration of PCM-Air heat exchangers as Thermal Energy Storage units for temperature maintenance in rooms. The methodology proposed is the use of design of experiments applied to numerical simulations on a theoretical model previously developed and experimentally validated. Although a theoretical model could be a useful tool for designers, such a design will not be sufficient if it is faced without a statistical approach. The proposed methodology is employed through the response surfaces in order to limit the number of simulation runs required to achieve an appropriate, or optimal, solution. When applied to the study case, this methodology shows an improvement of the proposed design compared to the one initially posed: the time to reach the threshold air temperature has been extended, the initial investment has been reduced, and the melting degree of the system has been improved; however, as a drawback, the TES unit volume has been increased. Furthermore, the proposed methodology has demonstrated to be a powerful tool to: reduce the number of numerical simulations runs and the invested time; improve the design; find an optimal point of operation; and find the factors settings that enable to fulfil with the requirements.

1. Introduction

When thinking of potential uses of Phase Change Material (hereafter PCM)-air heat exchangers one can consider any class of application directly related to the air at room temperature trying to take advantage of the temperature swing in the day/night natural cycle to facilitate the melting and solidification of PCM. In this work we study the design and integration of this type of Thermal Energy Storage (hereafter TES) unit for temperature maintenance in rooms. The methodology proposed here is the application of design of experiments (hereafter DOE) applied to the numerical simulations [1] on a theoretical model previously developed, by means of the response surfaces [2, 3]. Thus, achieving significant savings on the time spent on the design [4], if similarity relationships between the prototype and the model are met. The theoretical model used here numerically simulates the behavior of a TES unit based on the heat exchange between PCM and air [5]. Just after the experimental validation of the theoretical model is achieved, the combined technique is applied. To meet the requirements of the proposed study case, the application of the DOE methodology has been posed for a wider range rather than the experimental validity one. The calculation of the dimensionless relations of interest that characterize the equipment operation is made for both the experimental equipment and for each of the simulated runs. So the degree of dimensionless similarity of the proposed equipment
with the experimental one is checked. Therefore the need for additional experimentation of the proposed unit can be stated. The aim of this paper is to go one step further trying to establish a methodology on how to design a PCM-air heat exchanger, particularly based on those with macroencapsulated PCM with plate shape. Specifically, the design and integration of the unit for temperature maintenance in rooms is studied.

2. Methodology

In order to appropriately design and integrate PCM-Air heat exchanger for temperature maintenance in a room, a pre-design stage was considered first: as a result of the experimental data analysis, an empirical model was developed to simulate the thermal behavior of the tested heat exchanger. Since the thermal properties of PCM vary with temperature, a PCM-air heat exchanger works as a transitory system and therefore, its design must be based on transitory analysis. Furthermore, the empirical model was used as a very first and fast approach to pre-design the TES unit as well as to check the technical feasibility of its incorporation into a system. Then, the combined technique proposed here was applied. The basis of this methodology is the theoretical model developed to numerically simulate the thermal behavior of a TES unit based on PCM-air heat exchange. Once the theoretical model was experimentally validated [6] the potential application of interest was selected and then the corresponding TES unit was designed under the proposed methodology of DOE applied to the numerical simulations.

2.1. Pre-design: empirical model

An empirical model was built from the experimental results. The aim was to simulate the thermal behavior of the tested heat exchanger in different cases. These simulations were used to evaluate the technical feasibility of the application. The model describes the temperature evolution of a room with an internal cooling demand, where the PCM-air heat exchanger is operating and there is a ventilation system. The enclosure temperature was considered to be the average between the outside temperature and the room temperature (the enclosure is the typical lightweight construction of telecom shelters: insulation material layer (glass fiber) between two plate metal sheets so \( T_{\text{enclosure}} \) “effect” is going to be very low). A diagram of the room is shown in figure 1. Eq. (1) shows the energy balance applied to the air inside the room.

\[
\begin{align*}
\Delta T & \text{ is obtained at each instant as a function of } T_{\text{surface}} \text{ and the inlet air temperature \( (at \text{ instant } i \text{ equal to } T_{\text{room}}) \); and the } T_{\text{surface}} \text{ at instant } i \text{ is obtained from the stored energy evolution. The real-scale PCM-air heat exchanger tested was constituted of 18 parallel PCM plates-wall. A module is constituted by a metallic PCM container between two air channels modules. The pressure drop is the same for each module, and the air distribution through the air channels can be considered uniform. The unitary air flow through a module is } m_{\text{air HX}} \text{ divided by 18. Since the geometry and the air flow were kept identical, } E_{\text{mod}} \text{ between two temperatures is the stored energy for the real-scale PCM-air heat exchanger between the two temperatures divided by 18 (Eq. (2)). The total melting time depends on } E_{\text{mod}} \text{ and on } Q_{\text{demand}} \text{ (Eq. (3)). In order to apply a modular design, the relation between the experimental heat rate provided by the electrical resistances to simulate the thermal load and the heat rate demanded in a potential application (} \dot{Q}_{\text{demand}} \text{) is established according to the experimental number of PCM modules (18) and the ones required for design (} \#_{\text{modules}} \text{).}
\end{align*}
\]
Figure 1. Schematic diagram of the room in which the temperature is evaluated

Stored energy = \#_{\text{modules}} \cdot t_{\text{stored}} \cdot E_{\text{mod}}

\begin{align*}
t_{\text{melt}} &= \frac{\text{Stored energy}}{\dot{Q}_{\text{demand}}} = \#_{\text{modules}} \cdot t_{\text{mod}} \cdot \dot{Q}_{\text{demand}} \cdot E_{\text{mod}}
\end{align*}

\begin{align*}T_{\text{plateau}} &= T_{\text{melt}} + 1.58 \cdot Q_{\text{resistances}} = T_{\text{melt}} + 1.58 \cdot \dot{Q}_{\text{demand}} \cdot 18 / \#_{\text{modules}}
\end{align*}

\begin{align*}\Delta T = 1.4683 - 1.10943 \cdot T_{\text{surface}} \cdot °C + 1.10706 \cdot T_{\text{inlet}} \cdot °C
\end{align*}

\begin{align*}T_{\text{melt}} &= T_{\text{ob}} - 1.58 \cdot \dot{Q}_{\text{demand}} \cdot 18 / \#_{\text{modules}}
\end{align*}

\begin{align*}\#_{\text{modules}} &= \dot{Q}_{\text{demand}} \cdot \Delta t_{\text{ob}} / E_{\text{mod}}
\end{align*}

The value 1.58 comes from the linear correlation between \( T_{\text{plateau}} \) and \( Q_{\text{resistances}} \) data obtained experimentally. The origin ordinate is the average phase change temperature of the PCM used. The relationship between \( T_{\text{melt}} \) and the cooling power demand is described in Eq. (4). Assuming that the origin ordinate in the adjustment Eq. (5) is \( T_{\text{melt}} \), it is possible to define the number of modules and the \( T_{\text{ob}} \) needed for a given cooling power demand, as well as the \( T_{\text{ob}} \) and \( \Delta t_{\text{ob}} \) to maintain such a level (Eqs. (6) and (7)).

The study case proposed following is the one stated by Lazaro [7] regarding temperature maintenance in a room (similar to a telecom shelter), which provides that, for proper running of the electronic equipment inside, the maximum air temperature in the room should be between 38 °C and 48 °C; in particular we will establish it at 44 °C. The heat generation of the electronic equipment is 5 kW. For the temperature evolution inside the room, an energy balance was stated with the following assumptions: 1) the cooling effect of the terrain was not considered. The ground floor area is supposed to be occupied by the equipment; 2) exterior ventilation is introduced only when it is favourable, and considering that the environment outside the room is 40 °C (as boundary condition specified by the company). The idea behind this system is that after a failure of the conventional cooling system, the TES unit is intended to smooth the evolution of the room temperature so that it extends the time to reach a certain threshold temperature. The aim is this period to be about two hours, so technicians have sufficient time to reach the place where the room is located and to repair the damage of the cooling system without having to stop the electronic equipment. The empirical model is used to provide a fast first approach of the technical feasibility of incorporating the TES unit in the selected application. If it fits, the second stage of design begins.
2.2. Improving design: Theoretical model, DOE applied to numerical simulations
The empirical model can give a very fast approach of relevant design parameters such as the PCM average phase change temperature. However, if we want to analyze the behaviour of the equipment when modifying any other parameter or variable, or if we need to improve/optimize the design, we have to move to the numerical model [6, 7].

2.2.1. Similarity analysis: scaling the model. To meet the requirements of the proposed study case, the application of the DOE methodology has been posed for a wider range rather than the experimental validity. Due to the specific requirements of the study case, the similarity relationships between the experimental equipment and the equipment proposed for the application will not be adjusted in all cases (model-prototype similarity). Thus, calculation of the dimensionless relations of interest that characterize the equipment operation is made for both the experimental equipment and for each of the simulated runs. So the degree of dimensionless similarity of the proposed equipment with the experimental one is checked. Therefore the need for additional experimentation of the proposed unit can be stated, in the case of not being within the experimental validity range.

2.2.2. Validity range. The experimental validity range has been established for a series of relationships that characterize the heat exchange process in the TES unit. All the ranges are gathered in Table 1. Specifically, the following ranges of values have been determined: the Reynolds number; the number of transfer units; the Biot number; and the thermal conductivities ratio ($\lambda_{\text{eff}}/\lambda$) that quantifies the effect of natural convection within the PCM inside the plate. As this relation goes beyond 1 the effect of natural convection is more substantial. These parameters stand to check that every proposed unit is within the experimental validity range. Their determination is detailed in Dolado [8], pp 115-118, and is based on the following main Eqs. (8-10) (where $T_1$ is the air temperature in the TES unit (average between the inlet and the outlet), $T_2$ corresponds to $T_{\text{melt}}$.

$$\lambda_{\text{eff}} = \lambda \cdot Nu$$  

$$N_{u_l} = 0.42Ra_l^{0.4}Pr_1^{0.1012} \frac{H}{L}^{0.3}, \text{ valid for } 10<H/L<40; \ 10^4<Ra_l<10^7; \ 1<Pr<2 \times 10^4$$  

$$Ra_l = g \beta \cdot T_1 - T_2 \cdot L / (\alpha \nu)$$

| Re  | NTU | Bi  | $\lambda_{\text{eff}}/\lambda$ |
|-----|-----|-----|---------------------|
| 917 | 2577| 0.013| 0.039 | 0.088 | 0.875 | 1.00 | 1.74 |

2.2.3. Application to the case study. As a starting point we will continue using the case brought by Lazaro [5]. A series of restrictions put on the TES system follow:
- Dimensions limitation due to the telecom shelter: the maximum length of the system is limited to 2.5 m (height of the shelter) which limits the section of the PCM to 1.25 m. Likewise, the width of the unit is also limited to 5 m due to the wall;
- Electrical power consumption limitation of the fan: so the fan can be electrically supplied by batteries without being essential a connection to the grid. Pressure drop should be less than 30 Pa.
- Operating conditions from the empirical model are to be considered inside their factor domains. For the implementation of DOE the following factors and responses were considered:
- Factors (listed in table 2 along with their domain): mass of PCM, air flow, air channel width, thickness of the PCM plate, finishing of the plates (related to rugosity or to the presence of bulges in the surface of the plates).
- Responses: melting ratio in 3 hours, additional time for the air to reach a temperature of 38 °C (compared with the evolution of temperature without unit TES) in the room, additional time for the air to reach a temperature of 44 °C (compared with the evolution of temperature without TES unit) in the room, pressure drop; initial investment (mainly depending on the amount of PCM, the installed fan, the casing, and whether or not the plates have bulges on its surface).

2.3. Response optimization

Given that the main objective of the TES unit is to extend the time period during which the room temperature is below a certain temperature limit, the highest importance has set to that response. Table 3 lists the input parameters in the optimization. It has been considered that the most important requirement is to get the unit to extend as much as possible the time to reach the temperature limit of the air in the room, assigning the greatest importance to the maximum temperature limit (44 ºC) and considering also important, but lesser, the time to reach the first temperature limit (38 ºC) as well as \( \Delta p \) (in order to be as lower as possible). Also the investment and the melting ratio are interesting responses considered in the study, as they are related to economical and technical feasibility respectively. Once the objectives are defined, each variable is assigned a weight (between 0.1 and 10) and an importance (also between 0.1 and 10). In this approach to the optimization, each of the values of the responses is transformed using a desirability function. The weight defines the shape of this function for each response and is related to the emphasis on achieving the target (a value greater than one emphasizes the importance of achieving the goal; a unit value gives equal importance to the objective and the limits; a value less than one puts less emphasis on the goal).

After calculating the desirability for each response, the desirability composite is calculated (weighted geometric mean of the single ones) that allows to obtain the optimal solution. In this case, the same weight is set to each of the answers assuming a unit value. This will set the target as important as any value within the limits for the corresponding answer. On the other hand, assigning a value to the importance of each answer is related to the importance given to each of the answers, and if any of these responses is more important than the others (most important is a 10, less important is a 1).

### Table 3. Optimization parameters

| Response variable | Objective | Weight | Importance |
|-------------------|-----------|--------|------------|
| \( t_{\text{add} \ T=44^\circ C} \) | Maximize   | 1      | 10         |
| \( \Delta p \)     | minimize  | 1      | 5          |
| \( t_{\text{add} \ T=38^\circ C} \) | Maximize   | 1      | 5          |
| Investment        | minimize  | 1      | 1          |
| \%Melt            | Maximize   | 1      | 1          |

3. Results and discussion

3.1. Empirical model results

Technical feasibility of incorporating the TES unit in the shelter for temperature maintenance is checked first with the empirical model. Figure 2 shows that, taken into account the boundary conditions shown in table 4, a reduction of the air temperature in the room can be provided with the TES unit, increasing significantly the time to reach the threshold temperature.
3.2. Theoretical model results: DOE & numerical simulations
Once the viability is checked, the theoretical model comes into play. The operating conditions of the unit proposed by Lazaro [5], as well as the main simulation results obtained with the theoretical model are shown in table 5.

**Table 4. Boundary conditions Lazaro’s case**

| $Q_{demand}$ [W] | $T_{room}$ [°C] | $V_{radiation}$ [m$^3$/h] | $T_{outside}$ [°C] | $m$ [kg] | $c_p$, envelope (glass fiber) [J/(kg*K)] | $T_{room}$ at $t=0$ [°C] |
|-----|----------------|---------------------------|-------------------|---------|---------------------------------|----------------|
| 5000 | 27             | 2500                      | 40                | 2180    | 880                             | 20             |

**Table 5. Operating conditions and Main results of the simulation with Lazaro’s case**

| Operating conditions | Results |
|----------------------|---------|
| $M_{PCM}$ [kg] | $V$ [m$^3$/h] | $c_{plate}$ [mm] | $c_{air}$ [mm] | Finishing | $%Melt$ | Investment [€] | $t_{add}^{T=38^\circ C}$ [min] | $t_{add}^{T=44^\circ C}$ [min] | $\Delta p$ [Pa] |
| 132 | 1340 | 6.5 | 12 | 3 | 69.47 | 3924 | 36 | 63 | 36 |

3.3. Optimization
Then, the combined technique is applied in order to optimize the design. What is interesting of the optimized results (figure 3) is the value of composite desirability as well as its trend according to each of the factors considered. The composite desirability obtained in this case (0.919) indicates that the values determined by the optimization nearly fulfil the requirements of the response variables. The trends of composite desirability for each factor allow to adjust their value (usually due to physical or technological constraints) while keeping high desirability values. However, at least there are two drawbacks to use this configuration: first, it does not respect the width limitation (this unit has a width of more than 10 meters), and secondly, when manufacturing the TES unit it will be more feasible to use a PCM thickness higher than 0.5 mm (proposed in the optimization). Thus, moving in the optimization plot to a greater value of PCM thickness without reducing too much the composed desirability and rounding parameters, a value of 2.5 mm in thickness is selected (which meets the width restriction). Results of the last proposed unit (table 6) are somewhat unfavourable compared to the optimized unit, but the proposed PCM thickness is much more realistic. Yet responses provided by the proposed unit represent a storage that improves every aspect of the very first one but the volume.
Figure 3. Optimization plot results (each subplot shows a curve with the corresponding desirability function; vertical red line shows the current value; blue slash line crosses with each desirability function in the optimal point; grey zones delimit the zero desirability zone)

Table 6. Main results of the proposed and optimized units

| Unit   | %Melt | Investment [€] | $t_{add\ T=38³C}$ [min] | $t_{add\ T=44³C}$ [min] | $\Delta p$ [Pa] |
|--------|-------|----------------|--------------------------|--------------------------|-----------------|
| Proposed | 92.64 | 3489           | 37                       | 73                       | 5               |
| Optimized | 100   | 3234           | 60                       | 96                       | 3               |

3.4. Model-prototype similarity
Dimensional analysis of these units show that the natural convection within the PCM is not going to be significant in any of the 2 units (proposed and optimized), being the heat transfer process by pure conduction for the second unit, and $\lambda_{eff}/\lambda$ within the validity range of for the other one [8]. Since both Re, Bi and NTU are within the experimental validity range, the units can be used for design purposes.

4. Conclusions
The combined methodology of DOE applied to the numerical simulations seems to be a valid tool for design this kind of heat exchangers. When applied to the case study of temperature maintenance in a room, time to reach the maximum air temperature in the room was increased (19.7%), the initial investment was reduced by 11% and the PCM melting ratio was improved by 23.2%, as a drawback, the volume occupied by the unit was increased around 3 times. This methodology shows an improvement of the proposed design compared to the one initially posed: the time to reach the threshold air temperature has been extended, the initial investment has been reduced, and the melting degree of the system has been improved; as a drawback, the TES unit volume has been increased.

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Nomenclature

\[ c_v = \rho c_p V \frac{\partial T}{\partial N_{wall}} \] [J/(s·K)], heat capacity

\[ c_p [\text{J/(kg·K)}], \text{effective specific heat} \]

\[ e \] [m], thickness of the PCM plate

\[ e_{air} [\text{m}], \text{air gap thickness between 2 PCM plates} \]

\[ E_{mod} [\text{kJ}], \text{total thermal energy stored in 1 module} \]

\[ g [\text{m/s}^2], \text{gravity acceleration} \]

\[ h [\text{W/(m}^2\cdot\text{K)}], \text{convection coefficient} \]

\[ H [\text{m}], \text{PCM plate height in vertical position} \]

\[ i, \text{time step in the numerical scheme} \]

\[ L [\text{m}], \text{PCM plate thickness} \]

\[ m [\text{kg}], \text{building enclosure mass} \]

\[ m_{air, HX} [\text{kg/s}], \text{air mass flow through HX} \]

\[ m_{ventilation} [\text{kg/s}], \text{ventilation air mass flow} \]

\[ M_{PCM} [\text{kg}], \text{PCM mass} \]

\[ N, \text{number of PCM plate walls inside storage unit} \]

\[ NTU = \frac{h A_x w}{C_v}, \text{number of transfer units} \]

\[ Q_{cond} [\text{KW}], \text{internal cooling demand} \]

\[ Q_{electrical} [\text{kW}], \text{heating power of the electrical resistances used in the experimental setup} \]

\[ t [\text{s}], \text{time} \]

\[ t_{melt} [\text{s}], \text{total melting time} \]

\[ t_{add, T=38^\circ C} [\text{s}], \text{elapsed time to reach 38}^\circ \text{C in room} \]

\[ t_{add, T=44^\circ C} [\text{s}], \text{elapsed time to reach 44}^\circ \text{C in room} \]

\[ T [^\circ C], \text{temperature} \]

\[ T_{surface} [^\circ C], \text{average surface temperature of PCM} \]

\[ T_{mean} [^\circ C], \text{average of air temperature during the plateau (period when the temperature is almost constant due to PCM effect), obtained either from the evolution of } T_{room} \text{ when simulated or from } \]

\[ T_{air, outlet} [^\circ C], \text{air temperature at storage unit outlet} \]

\[ T_{melt} [^\circ C], \text{average PCM melting temperature} \]

\[ T_{ob, \text{target}} [^\circ C], \text{air temperature plateau objective} \]

\[ V [\text{m}^3], \text{room air volume} \]

\[ \dot{V} [\text{m}^3/\text{h}], \text{volumetric flow} \]

\[ w [\text{m}], \text{width} \]

\[ \#_{modules}, \text{number of PCM modules in storage unit} \]

\[ %\text{Melt}, \text{ratio of PCM melted, percentage} \]

\[ \alpha [\text{m}^2/\text{s}], \text{thermal diffusivity} \]

\[ \lambda [\text{W/(m·K)}], \text{thermal conductivity} \]

\[ \lambda_{eff} [\text{W/(m·K)}], \text{effective thermal conductivity} \]

\[ \rho [\text{kg/m}^3], \text{density} \]

\[ \Delta p [\text{Pa}], \text{pressure difference} \]

\[ \Delta T = T_{air, inlet} - T_{air, outlet} [\text{K}], \text{temperature difference} \]

\[ \Delta t [\text{s}], \text{time step} \]

\[ \Delta t_{ob} [\text{s}], \text{plateau time objective} \]

\[ \text{HX, Heat Exchanger} \]

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