Numerical modelling and thermal simulation of PCM–gypsum composites with ESP-r

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Abstract

The aim of the present work is to refine the ESP-r system by incorporating phase change materials (PCMs) modelling. The behaviour of PCMs is modelled using ESP-r’s special materials facility. The effect of phase transition is added to the energy balance equation as a latent heat generation term according to the so-called effective heat capacity method. Numerical simulations were conducted for a multi-zone, highly glazed and naturally ventilated passive solar building. PCM-impregnated gypsum plasterboard was used as an internal room lining. The air, surface and resultant temperatures were compared with the no-PCM case and the diurnal latent heat storage effect was analysed. While this effect did not cause a considerable reduction in the diurnal temperature fluctuation, the PCMs did effectively store solar energy in the transitions periods. Additionally, the energy requirement at the beginning and end of the heating season was estimated and compared with ordinary gypsum wallboard. Within this comparison, the PCM composite solidification temperature was 22°C (i.e. 2 K higher than the heating set-point for the room). The results show that solar energy stored in the PCM–gypsum panels can reduce the heating energy demand by up to 90% at times during the heating season.

Keywords: Numerical modelling; Building simulation; Phase change materials; PCM–gypsum composite; Latent heat storage system

1. Introduction

At the present time, many designers are attempting to utilise innovative technologies to achieve low energy design solutions. Because of the inherent complexity, modelling and simulation is required to arrive at optimal parameter values and avoid technology conflict. The work reported in this paper was concerned with the modelling of phase change materials (PCMs) to create a heavyweight response as a contribution to passive solar design.

It is well known that the thermo-physical properties of the construction materials will have a strong influence on a building’s energy consumption. Within a passive solar design, the heat capacity of the inner wall layer is dominant. Traditional heavy-weight constructions can give rise to problems of excessive thermal mass and cost. Where traditional building materials are combined with an inner PCM layer, isothermal phase change can be employed to provide close space temperature control at acceptable cost. Effectively, the additional latent heat of fusion is used to increase the thermal capacity of the construction.

Thermal energy is generally stored as sensible or latent heat. In the former case, the temperature of the medium changes during charging or discharging of the storage, whereas in the latter case the temperature of the medium remains more or less constant since it undergoes a phase

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transformation. Benard et al. [6] have presented an experimental comparison of latent and sensible heat within thermal walls.

The utilisation of PCMs in active and passive solar buildings has been a subject of interest since their first reported application in the 1940s [7]. Any PCM composite will comprise two components: a chemical, organic or inorganic compound that undergoes a phase transition within some fixed temperature range) defined by Eq. (2), the Goodman transform [11] can be used to remove the temperature dependent, effective heat capacity, outside the differential operator by defining a new dependent variable:

\[
\frac{d\bar{T}}{dt} = \frac{\partial h}{\partial T} \frac{\partial \bar{T}}{\partial T} + g(\bar{T}, t)
\]

where \( T \) is the temperature, \( \rho \) the density, \( h \) the enthalpy, \( \lambda \) the conductivity and \( g \) the heat generation rate. When \( \frac{d\rho}{dt} = 0 \) and \( \frac{dh}{dt} = \frac{d\lambda}{dt} = \frac{dC_{\text{eff}}}{dt} \), Eq. (1) becomes:

\[
\rho(T) C_{\text{eff}}(T) \frac{dT}{dt} = \nabla \cdot [\lambda(T) \nabla \bar{T}] + g(\bar{T}, t)
\]

where \( C_{\text{eff}} \) is the effective heat capacity.

For the non-linear problem (in the phase change temperature range) defined by Eq. (2), the Goodman transform [11] can be used to remove the temperature dependent, effective heat capacity, outside the differential operator by defining a new dependent variable:

\[
\bar{T}(\bar{T}) = \frac{1}{C_{\text{eff}}} \int_{T_{\text{init}}}^{T} \rho(T) C_{\text{eff}}(T) dT
\]

where \( T_{\text{init}} \) is the heat capacity in the solid phase, and \( C_{\text{eff}} \) the heat capacity in the liquid phase. Eq. (2) can thus be rearranged:

\[
\rho(T) C_{\text{eff}}(T) \frac{d\bar{T}}{d\bar{T}} = \nabla \cdot [\lambda(T) \nabla \bar{T}] + g(\bar{T}, t)
\]

4. Numerical model

The ESP-r control volume approach was adapted to describe the physical elements of the PCM model using ESP-r’s zones and networks elements. This method also allows the adoption of variable thermo-physical properties [12]. Spaces, described by geometry, construction and operational data, are interconnected using network models that describe air and moisture flow paths. The complete numerical model, together with boundary conditions and imposed control, is then passed to a central solver.

The control volume formulation is obtained by integrating associated partial differential Eq. (2) over a small polyhedron control volume, \( V \), applying the mean value theorem and divergence theorem, with homogeneous material and uniform boundary at each surface. Eq. (2) thus becomes:

\[
\rho(T) C_{\text{eff}}(\bar{T}) V(T) \frac{d\bar{T}}{dt} = \nabla \cdot [\lambda(T) \nabla \bar{T}] + g(\bar{T}, \bar{T}) \tilde{g}
\]
where $\bar{T}$ is the average temperature of $V$, $\bar{g}$ the heat generation rate over the control volume and $\hat{n}$ the outward drawn normal unit vector.

Some initial applications of the effective heat capacity method within ESP-r are presented elsewhere [13,14].

5. Implementation in ESP-r

According to the control volume and the effective heat capacity method, the effect of the phase transition is added to the energy balance equation via material property substitution. Effective capacity is a highly non-linear function of temperature within the phase change temperature range. It can be substituted, however, by a linear relationship. Such an approach has been proposed for the thermal simulation of single PCM components [1,15].

Within ESP-r, PCMs were modelled using the concept of special materials [16]. Special materials were introduced to ESP-r as a means of modelling active building elements that have the ability to change their thermo-physical properties in response to some external excitation (e.g. electro-chronic glazings and photovoltaic components). The special material functions of ESP-r may be applied to a particular node within a multi-layer construction. Any node defined as a special material is then subjected to a time variation in its basic thermo-physical properties.

6. Problem definition

Within a building energy system, the most important feature of a PCM composite is its thermodynamic properties:

Table 1

<table>
<thead>
<tr>
<th>Material property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latent heat of phase change (kJ/kg)</td>
<td>45.00</td>
</tr>
<tr>
<td>Phase change temperature range (K)</td>
<td>1.00</td>
</tr>
<tr>
<td>Conductivity (W/(m² K))</td>
<td>0.35</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1000.00</td>
</tr>
</tbody>
</table>

Table 1: Properties of PCM-gypsum composite

Three, naturally ventilated, zones were established to represent a middle portion of a multi-storey office. The perspective view presented in Fig. 1 shows the superimposed natural ventilation scheme. Two symmetrical zones are separated by a third, centrally placed, buffer zone.

Passive solar buildings, with their large glazing areas, may give rise to thermal discomfort problems. Different strategies such as controlled blinds, passive cooling or additional thermal mass may be used to mitigate the problem. Within the present study, additional thermal mass is achieved through the application of PCM impregnated gypsum board. The storage of latent heat increases the thermal capacity of the construction, allowing it to store solar energy while maintaining near constant temperatures. Table 2 lists the describing parameters of the two main zones.

The thermo-physical properties of the partitions and the magnitude of the air flows were defined according to best practice guidelines. All external walls were constructed from 25 cm of massive, concrete slab isolated with 12 cm polystyrene from the outside (Fig. 2). The heat transfer coefficient for all external, opaque partitions was set to 0.30 and 1.3 W/(m² K) for windows.

![Fig. 1. View of the three-zone PCM building model.](image-url)
Table 2
West and east zones description

<table>
<thead>
<tr>
<th>Zone parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total volume (m$^3$)</td>
<td>50.00</td>
</tr>
<tr>
<td>Floor area (m$^2$)</td>
<td>20.00</td>
</tr>
<tr>
<td>External opaque area (m$^2$)</td>
<td>16.50</td>
</tr>
<tr>
<td>External transparent area (m$^2$)</td>
<td>6.00</td>
</tr>
<tr>
<td>Total PCM wallboard area (m$^2$)</td>
<td>57.00</td>
</tr>
<tr>
<td>Floor area/PCM wallboard area</td>
<td>0.35</td>
</tr>
<tr>
<td>Thickness of PCM panel (m)</td>
<td>0.012</td>
</tr>
</tbody>
</table>

Weather data for Warsaw (52°N) in 1982 was used to define the boundary condition for the simulations. This year corresponds to the hottest summer between 1976 and 1985. The average ambient air temperature from July to September is 19.24 °C and the total solar radiation is 1144.5 MJ/m$^2$. The period from the beginning of March to the end of November was selected for the analysis. The wind speed and direction determined the infiltration air flow through the openings, the magnitude of which were set to guarantee effective air flow rates in order to maintain the zone temperature not higher than 3 K above the ambient temperature. The casual gains from equipment, lights and occupants were set to zero in order to remove their impact on the simulations and so make the results interpretation easier. Continuous heating corresponding to a fixed zone air temperature set-point of 20 °C was defined.

First, simulations were conducted for the building without PCM composites. Initial calculations showed that the maximum resultant temperature recorded in the west zone was 33.6 and 31.8 °C in the east zone. Additionally, the overheating effect was noticed from 15 June to 15 September when internal temperatures exceeded 25 °C during the day and night.

Now, an interior lining made from 1.2 cm of PCM–gypsum composite wallboard was applied to all surfaces except the floors in the west and east zones. Based on the resultant temperature history obtained from the initial simulation, the melting temperature ($T_m$) was set to 21, 24, 27 and 30 °C. The solidification temperature ($T_s$) was assumed to be 1 K higher than the melting point (i.e. 22, 25, 28 and 30 °C, respectively). Each composite has the same value of latent heat of fusion given by 45 kJ/kg.

7. Numerical analysis

A 15 min time step was used within the simulations. The values of the resultant temperature, PCM node temperature and latent heat of phase change were saved at each time step. To aid the analysis, the histories of these parameters were presented in weekly time periods. Each period was chosen to correspond to a different value of the melting temperature and contains the beginning of the phase change (i.e. where the wallboard’s surface temperature exceeds the melting temperature). The selected periods were:

- $T_m = 21$ °C: 6–12 March;
- $T_m = 24$ °C: 27 March to 2 April;
- $T_m = 27$ °C: 23–29 May;
- $T_m = 30$ °C: 19–25 July.

7.1. Wallboard temperature

The history of the PCM composite’s surface temperature and internal node temperature compared with traditional gypsum board are presented in Figs. 3–6 for different values of the melting temperature. The internal surface is highly exposed to a daily temperature fluctuation and direct solar radiation. The phase change process inside the wallboard allows a portion of the solar energy to be stored as latent heat. The surface temperature is about 0.5–1.0 K lower than for the case with no PCM–gypsum composites. This result is due to the relatively wide (~1 K) phase change temperature range in comparison to the daily zone temperature fluctuation (~2 K). The internal face of the wallboard (Figs. 7–10) is thermally stable and the temperature is constant at the level of the assumed melting temperature.
more pronounced temperature fluctuation is seen for the ordinary material, where the node temperature varies more than 1 K during 24 h.

7.2. Resultant temperature

The thermal behaviour of the wallboards also affects the room’s resultant temperature. Figs. 11–14 show the profiles over selected periods. An analysis of these data does not show significant differences in the zone’s performance. This derives from the relatively small thickness of the wallboard and the low latent heat of phase change (45 kJ/kg). The area of the wallboards is also relatively small on account of large glazed external walls, causing temperatures to rise significantly during the day. Another problem is that, from a practical point of view, the floor cannot be covered with a PCM composite and therefore its surface heats rapidly during the day; this impacts significantly on the room resultant temperature.
7.3. Latent heat storage effect

Figs. 15–18 show the history of the latent heat flux during transition periods. Over a day the heat flux is positive and solar energy is stored in the material (melting process). The heat is released during the night when the zone’s resultant temperature drops below the solidification temperature (solidification process). This process continues until the entire panel becomes loaded (i.e. the PCMs inside the porous media is completely melted and unable to store more heat).

The solar energy accumulated in the material is then equal to the maximum latent heat of phase change. For the cases studied only two PCM–gypsum composites attain the entirely loaded state (Figs. 19 and 20). In both zones (east and west) the composite with a melting temperature equal to 21 °C stores solar energy during March and releases it in November to cover the energy demands for heating. From April to October, the PCM panel is overloaded because the temperature is higher than the solidification temperature. The second type of composite, with a
melting temperature equal to 24°C, works similarly. However, now the loading period lasts 2 months and the material is overloaded for only about 4 months. Solar energy stored in the panel is utilized in October. The third material \((T_m = 27^\circ C)\) exceeds the fully loaded state for only a few days in the west zone, while in the east zone utilization is around 85%. The fourth material \((T_m = 30^\circ C)\) works periodically and provides no useful contribution for the case studied here.

7.4. Heating energy demands

The latent heat stored in the PCM panel is expected to partially cover the heating energy demand at the beginning and end of the heating season. The most important feature of the material, which determines its usefulness, is the solidification temperature. The solidification point should be above, but relatively close to, the required internal air temperature. Therefore, the first composite, with solidification temperature equals to 22°C, is deemed to be the most suitable in this case.

Figs. 21 and 22 shows the heating loads for each zones, east and west, during March. The differences in both cases,
Fig. 16. Energy stored as a latent heat in PCM composite wallboard ($T_m = 24^\circ$C).

Table 3

<table>
<thead>
<tr>
<th>Zone</th>
<th>Energy demand (kWh)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>March</td>
</tr>
<tr>
<td>No PCM East</td>
<td>22.11</td>
</tr>
<tr>
<td>$T_m = 21^\circ$C East</td>
<td>21.69</td>
</tr>
<tr>
<td>No PCM West</td>
<td>34.96</td>
</tr>
<tr>
<td>$T_m = 21^\circ$C West</td>
<td>34.58</td>
</tr>
</tbody>
</table>

with and without the PCM panel, are negligible. In the spring, the wallboard panel is completely unloaded after the winter and does not contribute to the energy demand. Consequently, there are no significant differences in the heating energy delivered during March (Table 3). On the other hand, in the autumn (the second half of November) the solar energy stored in the PCM during the summer significantly reduces (by more than 90%) the total heating energy requirements. The differences in heating loads are outlined in Figs. 23 and 24. In all zones with ordinary gypsum plasterboards, the heating system works continuously

Fig. 17. Energy stored as a latent heat in PCM composite wallboard ($T_m = 27^\circ$C).

Fig. 18. Energy stored as a latent heat in PCM composite wallboard ($T_m = 30^\circ$C).

Fig. 19. Solar energy utilised in PCM composite wallboard in east zone, with different melting temperature from beginning of March to the end of November.
Fig. 20. Solar energy utilised in PCM composite wallboard in west zone, with different melting temperature from beginning of March to the end of November.

Fig. 21. Heating loads in east zone with and without PCM wallboard in March.

Fig. 22. Heating loads in west zone with and without PCM wallboard in March.
from the middle of November. In the zones with PCM panels, the heating system operates periodically and only for short periods during the night.

8. Conclusion and future work

The results of a numerical analysis have confirmed the correctness of a proposed PCM modelling method. The histories of the zone’s resultant temperature and the wallboard’s surface temperature show the influence of the phase change transition and the effect of latent heat storage. Comparative analyses with pure gypsum plasterboards show the advantages of latent heat storage systems, indicating promise for the future.

This study is a contribution to the integration of latent heat storage materials within buildings. The initial model, implemented in ESP-r, to calculate the effect of phase change performed as expected but further refinements are required. The obtained results show the effect of latent heat storage on the thermal behaviour of the building. While this effect did not cause a considerable reduction in diurnal temperature fluctuation, it did decrease the internal air temperature in the seasonal transition periods when the solar energy was effectively stored. The PCM–gypsum composite designed for passive solar heating works properly under spring-autumn weather conditions and allows the stored energy to be utilised at the beginning of the heating season, resulting in a considerable reduction in heating energy demands. However, to design the appropriate material properties for passive heating during winter, and cooling during summer (i.e. long-term heat storage systems), a wider analysis using multicriterion optimisation is required. While the behaviour of the material composite corresponds to the experimental measurements, further macro-scale experiments are necessary to validate the model. Additionally, a more accurate description of the PCM structure with variable density and conductivity is planned.
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References