Modelling the thermal behaviour of a precast PCM enhanced concrete cladding panel

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ABSTRACT: To enable governments to comply with the European Directive 2010/31/EU on the energy performance of buildings, strategies are required to improve the energy efficiency of buildings. Using the mass of a building to store or dissipate heat can reduce the demand on the auxiliary heating and/or cooling systems and hence reduce the overall energy demand of the building. Previous research by the authors has shown that the incorporation of phase change materials (PCMs) into concrete enhances its thermal storage capacity by up to 50%. Precast cladding panels formed with PCM enhanced concrete have been developed and manufactured. Three full-scale demonstration huts were constructed using the panels and instrumented to record thermal data over an 18 month period. Analysis of this data showed that in particular environments the PCM-concrete composite is effective at reducing the air temperature in the huts and mitigating against overheating. Different building types will require bespoke optimal solutions for the application of a PCM composite material as a thermal energy storage system. For this reason the development of numerical simulation tools is necessary to achieve a practical and economic application of this technology. One of the main challenges of developing models for PCM composite materials is defining the dynamic thermal properties of the material during the phase change transition. This paper describes the development of a 2D finite element model using COMSOL Multiphysics in which the model is validated by comparing the simulated temperatures in the model with the actual temperatures recorded at the corresponding locations in the demonstration huts. The aim of the model is to validate the definition of the thermal properties of the PCM-concrete composite so that they can be used to model the thermal behaviour of the composite in any real situation.

KEY WORDS: Thermal Energy Storage; Phase Change materials (PCM); COMSOL Multiphysics; PCM-concrete composite

1 INTRODUCTION

According to the World Business Council for Sustainable Development [1] there is currently a stock of more than 80 million buildings in Europe built between 1950 and 1975, a period during which energy performance was not considered in building design. Often these buildings are fit for purpose structurally however their energy performance is very poor.

In order to achieve an improved energy performance while minimizing associated material consumption, a proposed solution is to retain the loadbearing structure but replace the non-loadbearing façade of the building with a modern, energy efficient building envelope. Improving the energy performance of building envelopes can reduce the sector's total energy consumption by 20% [2].

One of the most commonly proposed methods of enhancing the energy performance of a building is to use the mass of the building envelope to store thermal energy temporarily. This absorption and storage of heat during the day can reduce overheating of the internal environment in a building and hence reduce the energy demand of the air conditioning system. The stored heat is then dissipated into the internal environment at night when the temperature of the building naturally reduces. This use of thermal energy storage improves the thermal comfort of the occupants by moderating internal temperature fluctuations while also shifting electricity consumption to off-peak periods.

Previous research carried out by the authors [3 - 5] has shown that the thermal mass behaviour of concrete can be enhanced by incorporating phase change materials (PCMs) into the concrete which provide an additional latent heat capacity and hence increase its overall thermal storage capacity. PCMs are materials that absorb and release high quantities of heat energy at specific temperatures as they reversibly change phase, that is, from solid to liquid or from liquid to gas.

The previous research studies [3 - 5] found that PCMs can add significant thermal storage capability to concrete - up to 50% - augmenting its inherent thermal mass potential. This research also highlighted the fact that the effectiveness of the PCM in increasing the overall thermal storage of the concrete panels reduces with depth into the panel. This is due to the fact that the PCM absorbs the heat as it changes phase and hinders the penetration of heat deeper into the panel. The overall thermal storage of a panel will increase as the amount of heat energy transferred to the panel increases. In a real application where a PCM-concrete composite material is used in a building to store thermal energy, the effective depth of the PCM will depend on the temperature profile of the internal environment.

The analysis of heat transfer within PCM composite materials is very challenging due to their complex thermal behaviour which is influenced by several varying parameters. When selecting the PCM material for a building application the literature on this topic concludes that the melting/freezing temperature of the PCM should coincide with the desired internal room temperature. However for the PCM to have a positive effect on reducing the energy use in a building, it is critical that the air temperature in the location where the PCM is located fluctuates sufficiently within a 24 hour period to ensure that the PCM material changes phase. Many factors influence this requirement including the thermo-physical properties of the PCM and the material it is embedded in, along with the local climate, building geometry and use of the building. As all buildings differ, each building will require a unique optimal solution for the application of a PCM composite material as a thermal energy storage system. For this reason the development of numerical simulation tools is necessary to achieve a practical and economic application of this technology. Coinciding experimental data is required to validate a PCM numerical model.

For this reason, further research was carried out by the authors [6] in which cladding panels were designed and manufactured using PCM enhanced concrete. Three full- scale demonstration huts were constructed using the panels and instrumented to record internal thermal behaviour. Thermal data has been recorded at the huts over an 18-month period in order to observe the thermal behaviour of the PCM-concrete composite during all seasons. The data collected in the huts will enable a calibrated model to be developed that can accurately predict the response of the PCM composite in a full scale scenario. This model can then be used to predict the impact of the PCM-concrete composite material in any scenario. This paper describes the initial stages in developing a model to replicate the thermal behaviour of a PCM-concrete composite material using COMSOL Multiphysics software.

2 METHODOLOGY

Although there is a body of research that investigates the properties and thermal behaviour of PCMs within concrete, there has not been any significant research carried out into the effectiveness of the PCM-concrete composites in a full scale scenario and there has been no such studies carried out in climate conditions similar to Ireland. Also, to date, the thermal behaviour of a PCM-concrete composite has not been modelled in a full-scale scenario. For authentication of such a model it is important to have real data collected from a full-scale test in order to calibrate the model. This section describes the design of the full-scale test set up for collection of real thermal data which is then used in the development of a finite element model to predict the thermal behaviour of a PCM-concrete composite.

The design, manufacture and full scale monitoring of thermal behaviour of the precast PCM enhanced concrete cladding panel was part of a European funded Horizon 2020 project entitled IMPRESS (http://www.project-impress.eu). Partners in this project included a leading concrete cladding company, Techrete Ltd and Sirus International who provided the monitoring equipment in the huts.

2.1 PCM-Concrete composite

The PCM-concrete material was formed by adding a micro-encapsulated paraffin PCM product, named Micronal, to a self-compacting CEM I based concrete mix, with a dosage of 5% by weight of concrete. This dosage of Micronal in concrete has been shown to be the optimum quantity of Micronal to be used in a concrete mix application [7 and 8]. Higher quantities of Micronal yield impractically low concrete strengths and also causes significant reduction in the thermal conductivity and density, which tends to counteract the increase in thermal storage capacity. The mechanical and thermal properties of this PCM-concrete composite material were evaluated in previous research by the authors [4].

2.2 Design of the panels and demonstration huts

Three different types of panels were designed and manufactured for use in three separate test huts. Each panel comprised of a 70mm thick concrete outer leaf, 120mm insulation and a 125mm thick inner leaf which varies in composition (Figure 1). This study is investigating the thermal behaviour of the inner leaf of the cladding panel. As there is a 120mm layer of insulation between the inner and outer layer, the form of the outer layer has an insignificant effect on the thermal behaviour of the inner layer. Kingspan Kooltherm K15 Cladding Board was used for the insulation layer. This product is a high-performance rigid insulation with a thermal conductivity of 0.02W/mK

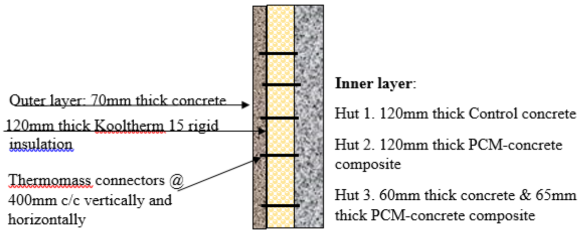

Figure 1. Summary of panel design for huts

For the Control hut, the inner leaf was constructed using a CEM I concrete mix without any PCM. For the second hut, the 120mm inner leaf of the cladding panel was formed using the PCM-concrete composite mix, as described in section 2.1. This hut is referred to as the Full-PCM hut. In the third hut, the inner leaf of the cladding panel was made up in two layers. The inner 60mm comprised of the PCM-concrete composite and the outer 65mm of the inner leaf, adjacent to the insulation layer, comprised of normal concrete without any PCM content. This hut is referred to as the Partial-PCM hut. The purpose of the Partial-PCM hut is to enable the effective depth of the expensive PCM to be assessed.

In order to ensure that the data from each of the huts is comparable, all of the huts had identical design parameters including dimensions, level of insulation, air tightness, glazing and orientation. The huts were positioned in an open site to mitigate any overshadowing. All the huts were orientated with the glazed elevation facing south. As the huts were due to be demolished at the end of the project, the internal headroom was limited to 1.8m. The clear internal plan dimensions of the hut were 1990mm x 1990mm. In order to capture solar radiation, the southern façade of each hut was glazed with double glazed sliding doors. As this research study aimed to investigate the thermal mass behaviour of the walls of the huts, the roof slab and floor slab were thermally isolated by placing 120mm of rigid insulation on the inner surface. This ensured that the concrete roof slab and floor slab did not provide any substantial thermal storage capacity in the hut. The junctions between the roof/floor and the cladding panel were designed to omit any thermal bridging effects. The demonstration huts were constructed and located in Techrete Ltd (Figure 2).

Figure 2. Demonstration huts located in Techrete Ltd

2.3 *Instrumentation of the test huts*

To observe thermal behaviour, a data recording and monitoring system was designed. Each hut is instrumented for collection of temperature data and internal and external environmental data (Figure 3). Thermocouples were cast into the internal layer of all the panels, located at depths of 30mm, 60mm and 90mm. Thermocouples were also located on the internal and external surfaces of the inner leaf and also on the outer face of the insulation layer. Each set of 6 thermocouples were located at the centre of each panel, north elevation, east elevation and west elevation. There were two additional sets of 6 thermocouples located in the north elevation panel. In total there are 30 thermocouples in each hut to record the temperature throughout the depth of each wall. This number allowed for redundancy in case any of the thermocouples were damaged during the manufacture or installation of the panels. These thermocouples enabled the varying temperature profile throughout the depth of the wall to be determined at any point in time.

A heat flux pad was located on the internal face of the north wall in each hut to indicate the heat flow into and out of the wall at the surface. A type K thermocouple recorded internal air temperature and a HOIKI Z200 also recorded internal air temperature and relative humidity (RH) in each hut. The external temperature and RH were also recorded and an EKO MS-802 pyranometer was used to record solar irradiance.

Interconnected programmable controls on the 2kW heaters with the same on/off phases were installed in each hut. The purpose of the heaters was to enable a heat load pattern to be applied to the huts that replicates a particular scenario, such as an overheating problem.

The rate of increase of air temperature in both PCM huts is lower than in the Control hut [6]. The peak air temperature in the Control hut is consistently higher than the peak temperatures in the PCM huts, generally in the order of 1°C.

3 COMSOL MULTIPHYSICS MODELLING

The aim of this part of the research project is to develop a model that can accurately predict the thermal behaviour of a PCM-concrete composite material when it is placed in environments with various internal temperature profiles and also different external climatic conditions.

One of the challenges in modelling a PCM-composite material is characterising the thermo-physical properties of the PCM composite correctly. Usually differential scanning calorimetry (DSC) is used to characterise a pure PCM.

However, for DSC the sample size is very small, so it is not an appropriate method for characterizing the thermos-physical properties of such PCM composites [9].

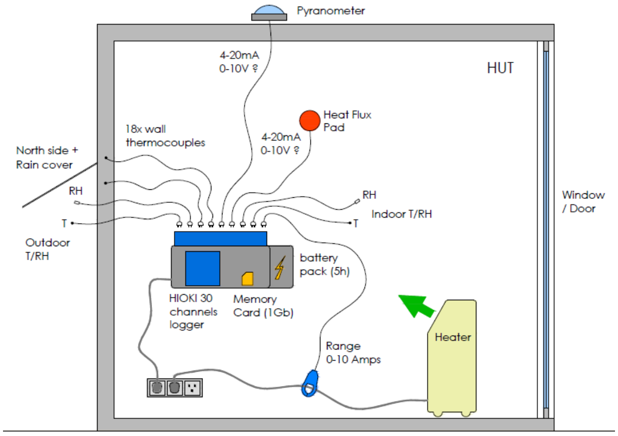

Figure 3. Schematic layout of instrumentation of each hut (Courtesy of Sirus)

3.1 *General formulation of the phase change problem*

The main feature of phase change problems is the moving boundary where the Stefan condition must be met, expressing the local velocity of a moving boundary as a function of quantities evaluated at both sides of the phase boundary. In problems of heat transfer with phase change, the physical constraint is that of conservation of energy, and the local velocity of the interface depends on the heat flux at the interface. For pure materials there is a clear distinction between the solid and liquid phases separated by a definite moving boundary at which melting occurs at a constant temperature. For conduction dominated heat transfer, as would be typical in a building application, the governing equations can be written for the solid and liquid phases respectively which have to be satisfied by the Stefan condition, as set out by Voller [10]:

Heat transfer in the solid phase:

$$\rho . C_s . \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s . \frac{\partial T_s}{\partial x}\right) \tag{1}$$

Heat transfer in the liquid phase:

$$\rho . C_l . \frac{\partial T_l}{\partial t} = \frac{\partial}{\partial x}\left(k_l . \frac{\partial T_l}{\partial x}\right) \tag{2}$$

The Stefan condition that enforces the heat balance at the solid–liquid interface is:

$$\frac{\partial}{\partial x}\left(k_s . \frac{\partial T_s}{\partial x}\right) - \frac{\partial}{\partial x}\left(k_l . \frac{\partial T_l}{\partial x}\right) = \rho . L . v \tag{3}$$

where:

ρ = density
C_s & C_l = specific heat capacity in the solid and liquid state respectively
T_s & T_l = Temperature of solid & liquid respectively
t = time
x = distance
k_s & k_l = Thermal conductivity of solid & liquid respectively
L = Latent heat of fusion
v = velocity of boundary

3.2 *Modelling of PCMs*

Numerical methods have been developed to model heat transfer during the solid – liquid phase change. The two most commonly used methods are the enthalpy method and the apparent heat capacity method.

The *enthalpy method* was proposed by Eyres et al. [11] to deal with variations of thermal properties with respect to temperature. The latent and specific heat are combined into a single governing equation. For conduction dominated heat transfer, equations (1), (2) and (3) are combined, where the latent heat is absorbed into the enthalpy term as follows:

$$\rho \frac{\partial H(T)}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \tag{4}$$

where H(T) is the enthalpy function which represents the total energy of the material including sensible and latent forms of energy.

The *apparent heat capacity method* was introduced by Hashemi and Sliepcevich [12] to solve one-dimensional heat transfer with phase change in the region that is a mix of solid and liquid phases. The apparent heat capacity method consists of solving the transient heat conduction equation (4) expressed in terms of temperature and specific heat $C_p(T)$.

$$\rho C_p(T) \frac{\partial (T)}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \tag{5}$$

Phase change materials for building applications, such as paraffin, melt or freeze over a temperature range compared to pure materials where phase change occurs at fixed temperature. This property makes the heat capacity method an attractive approach to simulating PCM in building applications [14 – 17].

The Heat Transfer Module in COMSOL Multiphysics uses the *Apparent Heat Capacity method* to model phase change materials. The latent heat is included as an additional term in the heat capacity. This method is the most suitable for phase transitions from liquid to solid, or solid to liquid.

As the melting and solidification of the PCM occurs across a temperature range, it is assumed that the transformation occurs in a temperature interval between $(T_{pc}-\Delta T/2)$ and $(T_{pc}+\Delta T/2)$ where T_{pc} is peak phase change temperature (24.4 °C for the Micronal PCM used in this project). The melt temperature range for the Micronal is 5.2 °C. The peak melt temperature range and latent heat (91 J/g) values for the Micronal were ascertained using differential scanning calorimetry. In this interval, the material phase is modelled by a smoothed function, θ, representing the fraction of phase before transition:

- $\theta = 1$ @ $T < (T_{pc} - \Delta T/2)$
- $\theta = 0$ @ $T < (T_{pc} + \Delta T/2)$

The density, ρ, and the specific enthalpy, H (heat absorbed or released), are expressed by:

$$\rho = \theta\rho_{sol} + (1-\theta)\rho_{liq} \tag{6}$$

$$H = 1/\rho\ (\theta\rho_{sol}.H_{sol} + (1-\theta)\rho_{liq}H_{liq}) \tag{7}$$

The apparent specific heat capacity C_p at temperature T for the PCM material is given by the equivalent heat capacity (ρH)+ latent heat, Kylili et al. [18]:

$$C_p = 1/\rho[\theta\rho_{solid}.C_{psolid} + (1-\theta)\rho_{liquid}.C_{pliquid}] + (H_{liq} - H_{sol})\frac{da_m}{dT} \tag{8}$$

where:

$$a_m = \text{mass fraction} = \frac{1}{2}.\frac{(1-\theta)\rho_{liq} - \theta\rho_{sol}}{\rho}$$

So the material properties for the solid and liquid phases are specified separately. These values are combined with the phase transition function so that there is a smooth transition from solid to liquid and vice versa, and the thermal behaviour during phase change can be modelled.

3.3 Modelling of PCM-concrete composite

The PCM-concrete composite material was modelled using the Heat Transfer in Porous Media module in COMSOL. The CEM I control concrete mix was used as the main material in the media. The density, thermal conductivity and specific heat capacity of this concrete had been previously determined in the laboratory. The volume fraction of Micronal that was added to the concrete was determined and set as the volume fraction of the porosity, that is, the volume fraction of pores filled with PCM, set as $(1-\theta_c)$, where θ_c is the volume fraction of concrete. Therefore, the effective thermal conductivity of the media was defined as:

$$k_{eff} = k_c\theta_c + k_{PCM}(1-\theta_c) \tag{9}$$

The subscript c refers to concrete.

Similarly:

$$(\rho Cp)_{eff} = \rho_c C_{p,c}\,\theta_c + \rho_{PCM} Cp_{,PCM}(1-\theta_c) \tag{10}$$

The PCM was modelled in accordance with equations (6), (7) and (8) using the Heat Transfer with Phase Change module within COMSOL.

4 RESULTS

4.1 Modelling of panel without PCM

Initially, a 2-dimensional model was created in COMSOL comprising of a 70mm thick concrete outer leaf, a 120mm insulation layer and a 125mm concrete inner leaf, reflecting what was used in the Control demonstration hut. The purpose of this initial simulation study was to investigate if the model is accurately simulating the heat transfer behaviour of the normal concrete.

Probes were located in the model corresponding to locations of thermocouples throughout the depth of the panels in the hut. The thermal properties for each layer were applied to the model, that is, density, thermal conductivity and specific heat capacity. The values of thermal conductivity, density and specific heat capacity for the concrete layers were taken from the results of the laboratory investigations (k_{conc} = 1.86 W/mK; ρ_{conc}=2335 kg/m^3; $C_{p,conc}$=881 J/kgK). Material properties for the insulation were taken from the Kingspan data sheet.

A simulation was run in which a 24 hour dynamic temperature profile of the internal wall surface in the control hut, from 8 am on 27th Dec to 9 am on 28th Dec 2017, was imported into the model and applied to the internal surface of the model panel. The initial temperature of the inner leaf was set at 18.7 °C because this was the temperature throughout the actual wall at the start of this time period. The heaters came on during this period and the temperature at the inside face of the wall increased to a maximum of 27 °C. The corresponding dynamic external air temperature data recorded during this period was also extracted from the hut data, imported to the model and applied to the external face of the model panel. The simulation calculated the temperature at each probe at five-minute intervals throughout the time period. The results of the simulation were plotted against the real temperature data recorded at each thermocouple in the control hut. It is beyond the scope of this paper to report on the full analysis of the simulation exercises, which included other time periods, however, a typical example of one of these plots is provided in Figure 4.

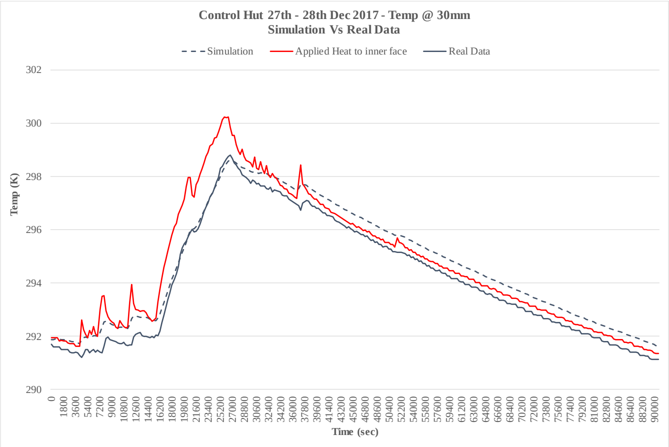

Figure 4 . Comparison of simulated temperatures and real temperatures at 30mm depth in Control hut wall.

An initial observations is that, generally, the thermal behaviour of the probes in the simulation follows a similar pattern as the actual thermocouples in the hut. There is a notable difference at the start of the simulation when the heaters are switching on and off about the set point – the simulation temperature rises quicker and is circa 0.5 °C higher than the actual temperature in the huts. When the heaters remain on continuously, the real and simulated temperature are similar. The slopes of the curves during the cooling period are very similar, albeit the simulated temp remains circa 0.5 °C higher than the real temp during the cooling period. Further sensitivity simulations were carried out to explore the effects of varying the input material properties. A parametric sweep was carried out in which the thermal conductivity of the concrete varied between 1.6 W/mK and 2.0 W/mK in increments of 0.1 W/mK, and the specific heat capacity of the concrete was varied between 750 J/kg and 1000 J/kg in increments of 50 J/kg.

4.2 Modelling of panel with PCM-concrete composite

The model as described in section 4.1 was adjusted to replace the material of the inner leaf of the panel with the PCM-concrete composite. A number of different 24 hour periods of real data collected at the Full PCM hut was selected for the simulation studies. During each period the internal air temperature increased sufficiently to ensure that some of the PCM within the depth of the wall would change phase. One particular period of interest was 23rd – 25th October during which the heaters were on for 6 hours during the day and then natural ventilation was provided at night to assist the discharge of heat from the internal walls (Figure 5). All parts of the wall increased in temperature above 20°C which is the temperature at which the PCM will start to melt. It can be noted that there was no difference in temperature between the back surface of the inner leaf and the thermocouple at 90mm depth indicating that the PCM was not engaged at 90mm.

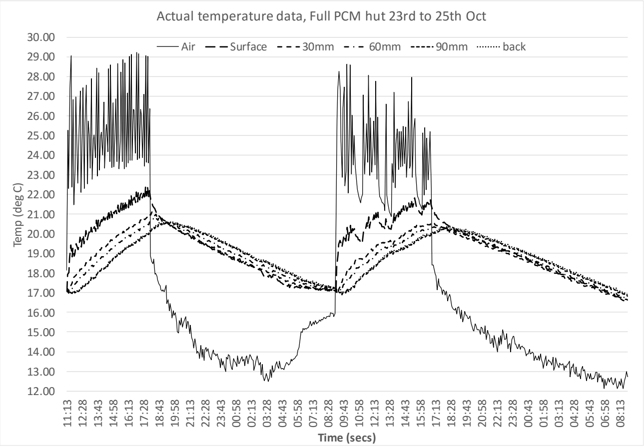

Figure 5. Real temperature data recorded in the Full PCM hut

The actual temperature profile recorded at the internal surface of the wall was applied to the internal surface of the 2-D model. The external temperature recorded during this period was applied to the external surface of the model panel. Figures 6 and 7 show comparisons between the simulated temperatures and real temperatures recorded at depths of 30mm and 60mm, and 90mm and 125mm respectively within the PCM-concrete composite wall.

The simulated and real temperatures follow a similar pattern with the maximum difference of circa 0.7 °C. It can be noted that the simulation temperatures increase at a faster rate during the heating period, while the rate of cooling is similar for both. It can also be noted that there is no difference in temperature between 90mm and 125mm depth in both the real data and the simulated data indicating that the PCM is not engaged at this depth for the heating load applied.

These observations may indicate that the thermal

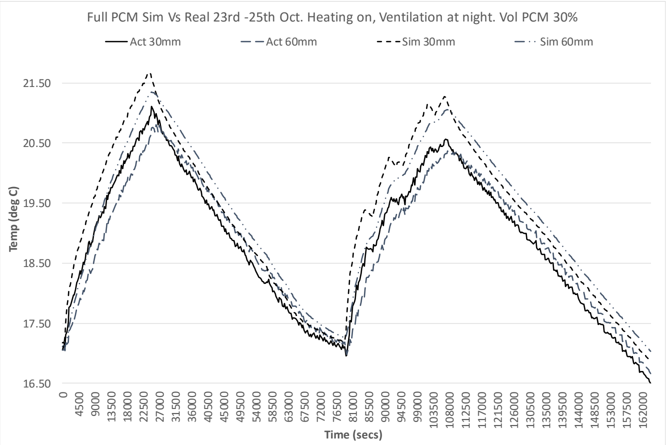

Figure 6. Simulation Vs real temperatures at 30mm and 60mm depths

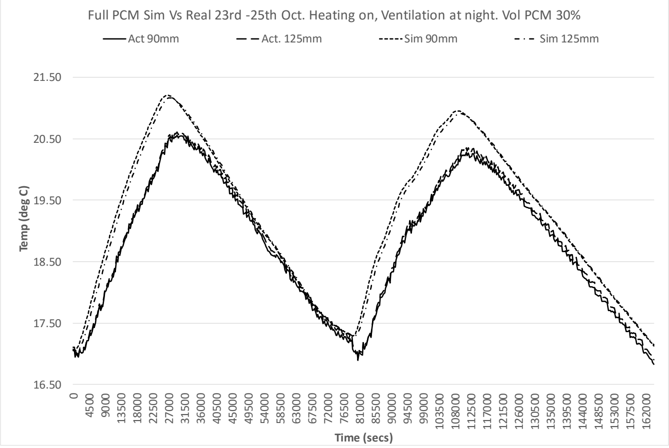

Figure 7. Simulation Vs real temperatures at 90mm and 125mm depths

conductivity of the PCM-concrete composite in the model is too high. However, a parametric sweep was carried out in which the thermal conductivity, the specific heat capacity, volume of PCM and peak melt temperature of the main matrix material, that is, the concrete, were varied. The results of this investigation showed that changing these did not improve the accuracy of the simulated results.

This type of modelling process has been carried out for a number of data sets taken from different weather seasons and applied heat load patterns, leading to differences between the simulated results and real data of no more than 0.5 ºC – 0.7 ºC.

5 CONCLUSIONS

COMSOL Multiphysics software was used to develop a model that can accurately simulate the thermal behaviour of a PCM-concrete composite material in a real life, full-scale scenario. The thermal properties of the PCM-concrete composite material were defined in the COMSOL model using a combination of *Heat transfer with Phase Change* and *Heat Transfer in Porous Media.* A 2-dimensional model replicating the concrete sandwich cladding panel used in a full-scale demonstration hut was created with the PCM-concrete composite used in the inner layer. Real temperature data, as recorded at the full-scale huts, was applied at the inner and outer faces of the model. Temperatures throughout the depth of the inner wall were extracted from the simulation and compared favourably with the equivalent real data recorded in the associated huts.

Initial results show that the model can simulate thermal behaviour of the PCM-concrete composite with reasonable accuracy, however, the rate of increase in temperature during a heating period is consistently greater in the simulated results.

A number of sensitivity studies have been carried out in which relevant parameters have been varied, however the difference between the rate of increase in temperature in the real data and simulated results is not significantly altered.

Further modelling work will be carried out to explore the influence of the thermal absorptivity and emissivity of the PCM-concrete composite on the accuracy of the simulated thermal behaviour.

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