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MODELLING THE THERMAL ENERGY STORAGE OF CEMENTITIOUS MORTARS MADE WITH PCM-VERMICULITE AGGREGATES

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Abstract

This paper presents a finite element modelling (FEM)-based approach to simulate the thermal performance and latent heat behaviour of sustainable cementitious mortars incorporating Phase Change Material–Vermiculite Aggregates (PCM-VAs). These advanced composites are designed to enhance thermal energy storage capabilities within building materials using porous vermiculite as a carrier medium for bio-based PCMs. An enthalpy-porosity formulation was adopted to solve the Stefan problem within the framework of coupled transient heat transfer, allowing for phase-change phenomena to be accurately captured across multi-scale domains. The FEM model was calibrated and validated using experimental data from an in-house testing program focused on optimized PCM impregnation techniques for vermiculite. The simulation results demonstrated good agreement with experimental measurements, effectively capturing the temperature evolution and storage-release cycles. This work supports the potential of PCM-VAs as a functional aggregate for low-carbon thermal regulation in cement-based construction systems.

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1. INTRODUCTION

The demand for energy-efficient and sustainable construction materials has increased in recent years, driven by growing environmental concerns and the need to reduce energy consumption in the built environment. A significant portion of energy usage in buildings can be associated with heating and cooling processes, prompting research into thermally adaptive materials capable of mitigating temperature fluctuations. Cementitious composites, while mechanically robust and widely used, inherently exhibit high thermal conductivity and limited thermal storage capacity, contributing to undesirable indoor temperature swings and higher energy demands for thermal comfort control. (Adesina, 2021; Haider et al., 2023; Jin et al., 2023, 2024; Krakowiak et al., 2020; Montazerian et al., 2023; Siddesh et al., 2025; Yang et al., 2023).

To overcome these limitations, researchers have investigated the incorporation of alternative aggregates and functional additives to improve the thermal behavior of concrete. Mineral aggregates, such as Vermiculite, have emerged as promising candidates due to their low thermal conductivity, high porosity. These materials can enhance the insulating properties of cement-based matrices, contributing to passive thermal regulation. However, their variable structure and potential incompatibility with cementitious environments raise concerns regarding durability and performance consistency. (Chin & Sih, 2018; Kumar et al., 2023; Mo et al., 2018; Neto et al., 2023; Schackow et al., 2014; Simpson & Stuckes, 1987).

Previous studies have largely focused on either experimental evaluations or numerical modelling of individual material modifications, with limited integration between approaches. Additionally, simplified models often fall short of accurately capturing the phase change dynamics and microstructural variability inherent in bio-based systems. (Abdolahimoghadam & Rahimi, 2024, 2025; El Majd et al., 2023; Liang et al., 2023; Liu et al., 2020; Nazari et al., 2020; Vitola et al., 2025).

In this study, both experimental and numerical methodologies were employed to investigate the thermal behavior of cementitious composites incorporating Vermiculite aggregates and phase change materials (PCMs). Spherical specimens were subjected to controlled thermal cycling, during which internal temperature profiles were continuously recorded. Concurrently, a computational thermal model was developed to simulate transient heat transfer within the composite elements.

This integrated experimental–numerical approach enables a comprehensive evaluation of the coupled effects of material composition and thermal response, thereby advancing the understanding required for the design of high-performance, energy-efficient, and sustainable building materials.

2. MATERIAL AND METHODS

The mineral clay, Vermiculite as an aggregates and carrier for PCM that used in this study is Lucky reptile vermiculite product (see Figure 1). The phase change material (PCM) employed was an organic PCM, RT-24 by Rubitherm characterized by a melting point near 24 °C and a latent heat of fusion of 180 J/g. The type of cement that is used is CEM II/B-LL 32.5 R as shown in Figure 1 is a type of limestone Portland cement characterized by its high initial resistance, produced by Heidelberg Materials at the Tavernola and Cagnano Amiterno cement plants. According to the composition prescribed by UNI EN 197-1, this cement comprises 65% to 79% clinker, with the remaining portion consisting of finely ground high-purity limestone with a Total Organic Carbon (TOC) content of no more than 0.20% by mass.

Figure 1: Vermiculite lucky reptile and Cement CEM II/B-LL 32.5R

The incorporation of PCM into Vermiculite aggregates followed a multi-step procedure. Initially, the Vermiculites were dried in 100 ~ 110 °C for 24 hours. Then RT-24 was melted by thermal belt to be in liquid form and added to dried vermiculite to absorb completely by the clays as the Vermiculite has a high absorption about 373% of its volume. This mixture must be under thermal belt in 40 °C for at least 6 hours. After 6 hours the mixed ingredients must be cooled for 45 minutes. Hence, the mixed ingredients must be in fridge to PCM change the state to solid condition. This combination needs to be covered by a layer of cement to be preserved

Figure 2: The procedure of preparing mixture of Vermiculite with PCM.

as appropriate for the concrete mortar mix design. Adding cement to this mixture and then put them together to have our needed aggregates. At least for one week it must be cooled in fridge to be capsulated well (see Figure 2).

Two alterative heat-flux DSC methods, namely the dynamic and a stepwise method, have been considered for this purpose. The German Standards DIN 51005 and DIN 51007 have been considered as a reference to perform the DSC tests (generally applied for this test method to any kind of material), while the IEA standard procedure is followed to determine the heat storage capacity of PCM (Sam et al., 2020).

Characterizing the PCMs was done by measuring three cycles over three different temperature ranges: (i) solid phase (-20 to 10 °C); (ii) phase change/transition (melting and/or crystallization), (10 to 30 °C); and (iii) liquid phase (30 – 60 °C). Three ranges, that occur during the DSC heating/cooling tests, describe the typical enthalpy and specific heat capacity evolutions of non-isothermal PCM (Sam et al., 2020).

Each sample measurement consisted of 3 (DSC) cycles over the pre-defined temperature range (-20 to 60 °C). Particularly, the first cycle was performed to eliminate previous thermal histories of the specimen; the second cycle was carried out to identify the TES characteristics; and finally, the third one was done mainly to check the reproducibility of the results and the possible appearance of cyclic chemical instability of the material (Sam et al., 2020).

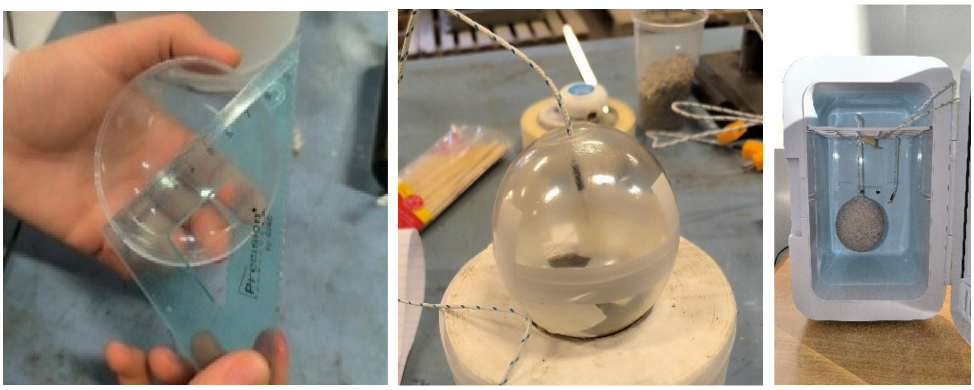

Figure 3: Left: DKK specimen diameter, Center: prepared mold; Right: sphere specimen inside the chamber.

A reference concrete mix was prepared using a mass ratio of 0.204:0.628:0.163:0.005 for cement, normal sand, water and superplasticizer respectively. Based on this control formulation, four concrete compositions were developed to assess the incorporation of vermiculite aggregates. In all modified mixtures, the normal sand was replaced by vermiculite aggregates at a 30% and 90% volumetric ratio. The formulations included: a reference mix (R) containing normal sand aggregates; a mix with vermiculite aggregates (VA); a mix using and a mix combining Vermiculite aggregates with embedded phase change material (VA-PCM). All mixtures were designed to maintain the same cement, allowing for consistent comparison of mechanical and thermal properties across the different formulations. Spherical specimen's samples (80 mm diameter) for thermal analysis (By DKK) test were cast (see Figure 3).

3. THERMAL ANALYSIS BY DYNAMIC SPHERE CALORIMETRY (DKK)

Temperature evolution measurements for all mixtures were conducted using specially prepared spherical samples which are considered as dynamic spherical calorimeters. The detailed preparation procedure and test method are described in a recently patented at the

Institut f¨ur Werkstoffe im Bauwesen – TU Darmstadt [23]. For each mixture, two spherical samples with a diameter of approximately 80 mm were produced. These thermocouples were positioned to measure the temperature evolution over time at the center of each spherical sample. The samples were placed inside a climate chamber (type IVYX Scientific) to measure temperature changes during heating and cooling phases. The temperature was monitored in the center of the spherical samples. The temperature range for the experiments was set between 10°C and 45°C. This testing method procured precise measurements of thermal properties of the mortar mixtures, providing valuable data on how additional aggregates influenced temperature evolution during both heating and cooling cycles. This information is critical to understand the thermal behavior and overall performance of the different mortar mixtures under varying temperature conditions see Table 1.

Composite	Cement	Sand	Vermiculite	Water	PCM	Superplasticizer
Reference	26.57%	66.53%	-	6.64%	-	0.26%
Vermiculite 30%	30.46%	53.37%	1.20%	14.67%	-	0.30%
Vermiculite 90%	48.03%	12.03%	5.68%	33.78%	-	0.48%
Ver 30% + PCM	26.30%	46.10%	1.20%	16.98%	9.16%	0.26%
Ver 90% + PCM	27.49%	6.88%	5.68%	32.84%	26.84%	0.27%

Table 1: Material's mass percentage for each composite mix

4. NUMERICAL MODEL

The basic equations, employed for predicting phase transformation phenomena in PCM cement-based systems, are described in this section. Modelling input is described on Table 2.

4.1. Thermodynamics principles

The basic equation describing a heat conduction problem can written as follows (see Eq. (1)):

$$\frac{\partial Q}{\partial t} = \nabla.(\lambda \nabla T) + \dot{q}_v \forall \boldsymbol{x} \in \Omega \tag{1}$$

where (Q) is the heat of the system, (t) the time, (λ) the thermal conductivity of the material (depending on temperature (T) and position vector $\boldsymbol{x}$ of the considered body Ω), $\dot{q}_v$ is the possible source term while $\nabla.$ and ∇ are the divergence and gradient tensorial operators.

In thermodynamics a small amount of heat added to a system (dQ) is defined by means of the first law of thermodynamics as Eq. (2):

$$dU = dQ - pdV \tag{2}$$

where dU is a variation of the internal energy of the system and pdV the rate of the work spent, indicated as dW (under the simplified hypothesis that $dW = pdV$).

By introducing the definition of the enthalpy of a homogenous system, $H = U + pdV$, and by combining Eqs. (1) and (2), and adopting the hypothesis of a constant pressure process, the following enthalpy-based equation can be reached Eq. (3):

$$\frac{\partial H}{\partial t} = \nabla.(\lambda \nabla T) + \dot{q}_v \forall \boldsymbol{x} \in \Omega \tag{3}$$

which is the mostly used equation for solving phase changes in construction and building material applications and is commonly addressed as the enthalpy-based method.

4.2. Enthalpy-based and Apparent Calorific Capacity Method

The Apparent Calorific Capacity Method (ACCM) allows for describing the enthalpy evolution of a system in terms of an apparent (or sometime called effective) heat capacity during the thermal phase change.

The approach is based on the following chain rule (see Eq. (4)):

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} \tag{4}$$

Then, by introducing the so-called temperature-dependent apparent (effective) heat capacity, defined as follows (see Eq. (5)):

$$\frac{\partial H}{\partial T} = \rho C_{eff}(T) \tag{5}$$

Eq. (3) modifies into the following non-linear transient heat Eq. (6):

$$\rho C_{eff}(T)\frac{dT}{dt} = \nabla.(\lambda \nabla T) + \dot{q}_v \forall \boldsymbol{x} \in \Omega \tag{6}$$

To complete the above problem statement of the ACCM approach outlined in Eq. (6), Initial Conditions (ICs) and Boundary Conditions (BCs) need to be employed.

Input Parameter	Symbol	Unit	Description
Thermal conductivity	K	W/m.K	PCM solid and liquid state
Specific heat capacity	C_p	J/kg.K	Varies with temperature
Latent heat of fusion and crystallization	L	J/g	Value obtained by PCM DSC test
Density	ρ	Kg/m3	-
Initial temperature	$T0$	°C	Based on DKK test parameters
Total simulation time	Δt	S	Based on DKK test parameters
Sample size	-	M	Based on DKK test parameters

Table 2: Input parameters and its description for studied numerical modelling.

5. RESULTS AND DISCUSSION

Figure 4 displays the temperature–time profiles of the concrete-based composites subjected to a controlled heating and cooling cycle, starting from thermal stabilization at 10 °C and progressing toward thermal equilibrium at approximately 45 °C. The curves represent the thermal evolution at the barycenter of the 80-mm diameter spheres made of distinct concrete formulations.

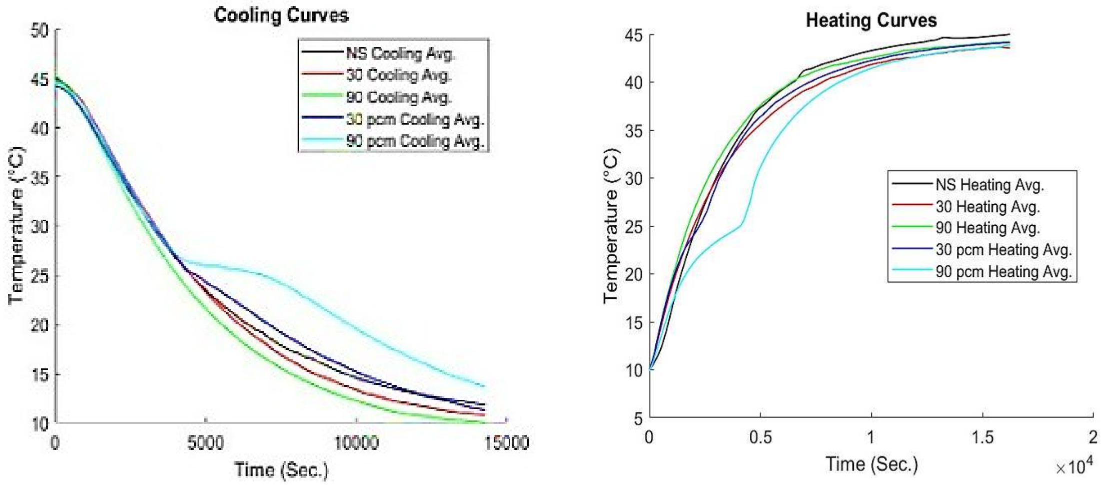

Figure 4: Thermal response of concrete spheres by DKK test with varying aggregate types during heating (right) and Cooling (left)

The heating cycle results revealed distinct thermal responses among the tested mixes. The reference sand mix heated rapidly and stabilized near 45 °C, reflecting high conductivity and low thermal inertia. In contrast, the vermiculate mixes (30% and 90%) showed slower heating and cooling, with the higher vermiculite content providing stronger insulation and greater heat retention. The PCM-enhanced mixes (30% + PCM and 90% + PCM) exhibited a characteristic plateau around 20–28 °C during both heating and cooling, corresponding to latent heat absorption and release. This phase change effect delayed heating and prolonged cooling, with the 90% vermiculite + PCM mix achieving the most pronounced thermal buffering due to the combined effects of insulation and latent heat storage. Overall, the findings confirm that vermiculite reduces heat transfer (insulation effect), while PCM provides latent heat storage (thermal storage effect). Their combination significantly enhances thermal inertia, making the 90% vermiculite + PCM mix the most effective configuration for passive thermal energy storage in building envelopes. The graphs in Figure 5 compare experimental data (heating and cooling) with simulation results for each formulation.

Reference specimen (NS, Figure 5a) has an excellent agreement between experimental and simulated curves, confirming well-calibrated thermal parameters, only minor cooling deviations, negligible in practice. 30% vermiculite mix (Figure 5b) has delayed heating and cooling due to low conductivity and porosity. Simulation captures heating well but underestimates cooling, likely from pore-related micro-resistances not represented in the model. 90% vermiculite mix (Figure 5c) has strongest insulating effect with extended thermal response. Simulation predicts faster behavior, suggesting overestimated conductivity/diffusivity; cooling mismatch reflects challenges in modeling highly porous composites. 30% vermiculite + PCM (Figure 5d) shows Phase change visible as plateaus. Experimental plateau broader than simulated, indicating greater latent heat and wider transition range; faster cooling in the model highlights need for refined PCM enthalpy/hysteresis representation. 90% vermiculite + PCM (Figure 5e) has longest response times from combined insulation and latent heat storage. Simulation reproduces the trend but underestimates plateau durations, leading to prematurely predicted phase change completion; deviations arise from reduced conductivity and extended PCM transition ranges not fully captured. Overall, the framework is validated for plain cement (NS, Figure 5a), but refinements, such as temperature-dependent conductivity, broadened PCM transition ranges, and hysteresis effects, are required for PCM–vermiculite composites (Figures 5d–5e), where insulation and phase change strongly influence thermal inertia.

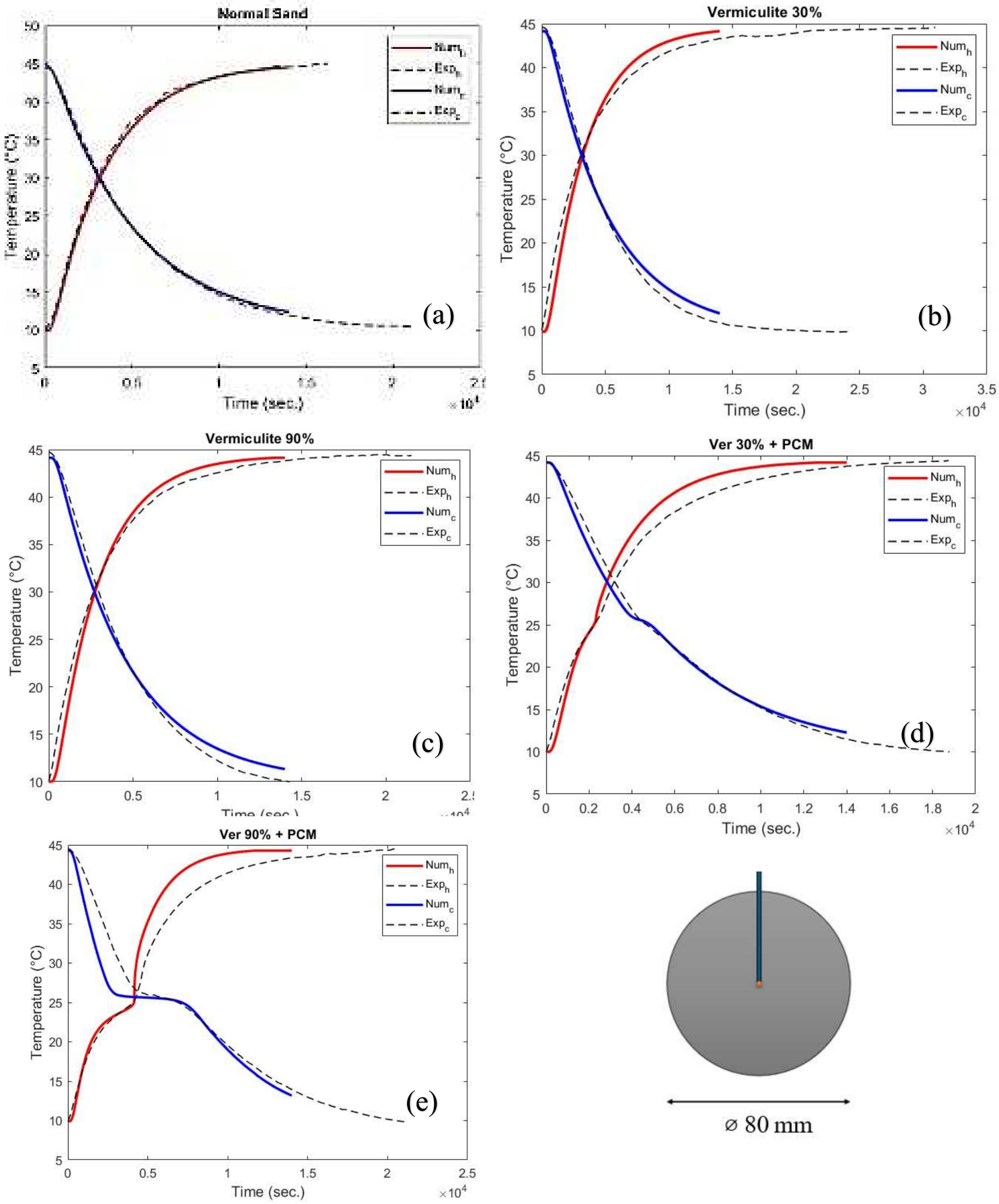

Figure 5:Curves extracted from experimental DKK tests vs. numerical results: (a) Reference concrete; (b) Concrete with Vermiculite 30%; (c) Concrete with Vermiculite 90%; (d) Concrete with Vermiculite 30% + PCM; (e) Concrete with Vermiculite 90% + PCM.

6. CONCLUSION

This study confirmed the feasibility of enhancing cementitious mortars with vermiculite and PCMs to improve thermal energy storage. DKK tests showed that vermiculite increases insulation by slowing heat transfer, while PCMs provide latent heat storage, prolonging heating and cooling cycles. The 90% vermiculite + PCM mix delivered the strongest thermal buffering effect. The finite element model reproduced the main thermal behaviors, with minor deviations for highly porous and PCM-rich mixes due to simplified assumptions and lack of hysteresis modeling. Overall, the experimental–numerical approach demonstrates the potential of PCM–vermiculite composites for sustainable building envelopes, with future refinements recommended in temperature-dependent properties and phase change hysteresis.

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