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RESEARCH ARTICLE

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Bio-based phase change material for enhanced building energy efficiency: A study of beech and thermally modified beech wood for wall structures

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Abstract

This study investigated the impregnation of beech and thermally modified beech (TMB) with a ternary mixture of capric acid, palmitic acid, and stearic acid as a bio-based phase change material (BPCM). Finite element method (FEM) was used to complement the experimental analysis by providing new insights into computational methods for simulating the behavior of BPCMs in untreated and TMB. The analyzed specimens namely beech and TMB were impregnated with BPCM; the TMB achieved 54% weight percentage gain (WPG) while untreated beech got 37%. Accordingly, a greater increase in the latent heat was obtained for TMB up to 90 J/g, while for untreated beech with BPCM up to 75 J/g. Impregnated specimens absorbed less moisture at relative humidity of air above 50%, likely caused by the high uptake and hydrophobic nature of the BPCM. The study highlights the research gap in performing mathematical simulations on wood samples with BPCM using material thermal properties derived from differential scanning calorimetry or T-History analysis. It shows that the direct use of these values for simulations leads to unacceptable outputs that result in high errors. The root mean square error for untreated and TMB samples impregnated with BPCM was in the range from 1.06 to 3.1 while that for untreated samples was in the range from 0.57 to 0.87, indicating that the main challenge in simulating and characterizing the samples is due to the interaction of the phase change material with the wood structure.

KEYWORDS

beech, finite element method; building constructions; latent heat storage; thermal mass, wood impregnation

1 | INTRODUCTION

As the world's energy demands continue to grow, the need for innovative and sustainable energy savings measures becomes increasingly important. One potential solution is the use of bio-based phase change materials (BPCMs), which can store and release thermal energy during phase transition.[1] BPCMs offer a promising approach for reducing energy consumption in buildings when implemented in the cladding and building structures.[2-6] By utilizing their ability to absorb and release heat, BPCMs help to stabilize indoor temperatures, which can lead to reductions in heating and cooling energy input.[4,7] When exposed to external heat sources, BPCMs undergo a phase transition from solid to liquid, absorbing excessive heat energy in the process. The energy is subsequently released back into the indoor environment when the external heat source is removed and the BPCM solidifies, providing a continuous thermal energy management system. By reducing the need for traditional heating and cooling systems, BPCMs not only help to lower energy costs, but also contribute to a reduction in carbon emissions, promoting a more sustainable approach to building design and operation. As in the European Union, the energy for heating and cooling indoor spaces accounted for 40% of the total energy consumption.[8] Phase change materials can be used in buildings to increase thermal mass, which is achieved by incorporating them into building materials typically used in lightweight construction, such as timber frame buildings. The principle of latent heat storage based on phase change materials can be applied to any porous building material.[9] Current research focuses on gypsum wallboards,[10] bricks,[11] cement-based composites,[12,13] and wood.[14]

Impregnation of BPCMs into wood has gained attention in recent years due to the excellent properties of wood as a building material, including its mechanical strength, low thermal conductivity, sustainability, and low density.[15-17] Due to the low density and high strength of wood, timber buildings have low total thermal mass. Phase-change materials in wood composites with working temperatures of 18°C to 25°C can absorb extra heat and release it when the temperature falls below a certain comfort point. Due to the wood porosity the BPCMs have great potential to increase the thermal mass of the wooden constructions and positively decrease the energy demand of the building for the indoor temperature regulations.[18] Solid wood with phase change materials can be effectively used as interior wall cladding or flooring to provide thermal storage around a building. Furthermore, the aesthetic appearance of the wood is preserved even after impregnation.[19]

Fatty acids are an option for incorporation into wood due to their natural origin and good compatibility with wood.[20,21] In addition, the fatty acid mixtures have high thermal stability. For example, research on pine wood impregnated with a mixture of capric and stearic acid showed only a slight shift in melting temperature and a decrease in latent heat after 600 cycles.[22] Moreover, other research conducted on delignified wood impregnated with capric acid and palmitic acid showed no difference after 100 cycles of cooling and heating of the composite.[23]

Although organic phase-change materials, such as those based on fatty acids, are more expensive than inorganic ones (eg, salt hydrates).[24] However, the use of biodegradable fatty acids may in the future reduce the price of post-use decomposition. Furthermore, fatty acids are not corrosive and show minimal changes in volume during phase change, which is advantageous when incorporating this material into a wood matrix. Other studies by incorporating capric acid and stearic acid into wood flour insulating material calculate a payback of the investment of BPCM composite for a maximum of 6 years in Turkey depending on the climatic region.[25] Previous studies have explored various impregnation parameters,[26,27] different wood species,[22,28,29] several BPCMs,[30,31] and techniques to improve the performance of the composite, for example, leakage through microencapsulation[32] or delignification and carbonization.[33]

Depending on the amount and type of BPCMs that can be hosted in the wood matrix, the latent heat of wood composites varies from 27 to 160 J/g.[14] The amount that can be embedded is related to the density of the wood. The higher the density, the lower the amount of BPCMs that can be incorporated. Beech and thermally modified beech (TMB) are increasingly used in European countries and is being implemented more and more in the construction sector. In the previous studies,[17,29] it was showed a possibility of impregnation of beech and TMB with BPCM based on coconut oil fatty acids. The highest latent heat of this BPCMs without wood was 122 J/g. Therefore, the present study aims to perform analysis of the incorporation of purer mixture of fatty acids having higher latent heat of 154 J/g[34] with a suitable working temperature for indoor use into beech wood and TMB wood. The analyzed BPCM is the ternary mixture of capric acid, palmitic acid, and stearic acid that has a melting temperature range around 23°C. The aim of the study is to investigate if the ternary mixture of fatty acid is compatible with the tested wood species, and their in-depth characterization, specifically with regard to their thermal behavior using two distinct techniques: differential scanning calorimetry (DSC) and T-history.[35] Additionally, this study utilizes numerical modeling simulations to complement experimental investigations and to elucidate the behavior of phase change materials namely the fatty acid mixture of capric, stearic, and palmitic acid in beech and TMB. Currently, there is a lack of suitable techniques to model the behavior of phase change materials when they are incorporated into bio-based materials as for example wood.[36] As the DSC or T-history analysis do not reflect fully the actual BPCM material behavior when incorporated into the wood, the novelty of this study lies in presenting a feasibility of digital model to predict the behavior of the material embedded in wood. The objective is to find out how this material performs and to highlight what are the factors that influence the accuracy based on the thermal properties results of beech and TMB with BPCM obtained by DSC or T-history analyses. That should be in the future analyzed in more detail. Furthermore, a possible solution to improve the reliability of the results is proposed.

2 | MATERIALS AND METHODS

2.1 | Materials

Capric acid (98%, Sigma-Aldrich, USA), palmitic acid (98%, Thermo Scientific, USA), and stearic acid (97%, Acros Organics, Belgium) were used in the study. Untreated and thermally modified by thermo-vacuum process at 210°C beech sapwood (*Fagus sylvatica* L.) devoid of visible defects (such as knots or cracks) were selected for the impregnation. The specimens were cut into dimensions of 9 × 90 × 90 mm prior to impregnation with the BPCM. The moisture content of the untreated specimens was 10%, while that of the TMB was 5%.

2.2 | Methods

2.2.1 | Impregnation process

A ternary fatty acid mixture, later named bio-based phase change material (BPCM), was prepared with weight ratios of 80% capric, 10% stearic, and 10% palmitic acid, respectively. The pre-weighed fatty acids were heated until they reached a liquid state and mixed thoroughly. To ensure homogeneity, the mixture underwent three cycles of freezing at 0°C and melting at 60°C.

The BPCM and wood specimens (five specimens per batch) were preheated for 30 minutes at 50°C, and impregnated in an autoclave. A vacuum of 350 mbar was applied for 10 minutes, followed by pressure of 6 bar for 1 hour. After releasing the pressure, the specimens were left in the mixture medium for 30 minutes at 50°C to reach equilibrium of pressure inside the specimens. After removing the specimens from the liquid, they were placed into an oven at 100°C for 3 hours. Afterwards, excess BPCM was wiped off with paper and the specimen's weight was recorded.

The weight percentage gain (WPG) was calculated as the difference between the initial and final weight of the specimens divided by the initial weight. To assess the effectiveness of the impregnation process, the maximum theoretical mass of PCM that can be incorporated into wood was calculated according to Hartig et al.[28] For the calculations, an approximate density of the PCM of 980 kg/m^3 (according to Duquesne et al.[24]) and the density of cell wall of 1500 kg/m^3 were taken. The specimens (five specimens of each type) were leached in an oven at 40°C for 72 hours and the rate of leakage calculated.

2.2.2 | Moisture interaction

Three specimens of each treatment were subjected to varying relative humidity (RH) to investigate the material interaction with moisture. The specimens were placed in a climate chamber at a temperature of 23°C and three levels of RH (25%, 50%, and 75%). The wood moisture content was deemed constant when the mass difference between two successive measurements taken at 24-hour intervals was less than 0.1%. The difference in moisture absorption between 50% and 25% RH and 75% and 50% RH was calculated to compare the moisture uptake of the samples impregnated with BPCM. The mass increase was calculated by subtracting the mass of the wood before impregnation to exclude the additional mass of the BPCM.

2.2.3 | T-history

The T-history method, described in reference 29 was used to measure and calculate the thermal properties of wood containing BPCM and control specimens without PCM simultaneously.

Specimens with dimensions of 9 × 90 × 90 mm and a copper plate of identical dimensions were tested, and K-type thermocouples were used to measure temperature changes. The specimens and reference were thermally insulated with 10 mm thick Armaflex (Armacell, Germany) material, and the thermocouples were placed at the centerline and middle of the specimens. The temperature change was recorded during 200 minutes at cold (0°C) and warm (40°C) ambient climates.

2.2.4 | Differential scanning calorimetry

DSC was performed using a DSC3 (Mettler-Toledo, USA) instrument under a nitrogen atmosphere to determine the thermal properties of the fatty acid mixture and impregnated wood specimens. Aluminum crucible pans were used to hold specimens weighing between 20 and 30 mg. The DSC tests were performed by subjecting the specimens to a heating and cooling rate of 2°C/min in the temperature range from 0°C to 40°C. This cooling-heating cycle was repeated three times for each specimen.

2.2.5 | Finite element simulation

Numerical analyses based on the finite element method (FEM), was conducted using ANSYS (2022 R2) software environment via ANSYS Workbench programming interface. The experimental temperature measurements from T-history analysis were used to validate the simulation results. The analyses considered untreated and specimens impregnated with BPCM. Transient thermal analysis was employed in all simulations, with the thermal conductivity of the wood specimens determined via the guarded hot plate method (Table 1). The specific heat capacity of untreated specimens was applied as report in Table 1. Moreover, enthalpy values, obtained through DSC analysis and T-History method, were incorporated into the material properties of the specimens.

A simplified two-dimensional model, sizing 90 × 9 mm as in the experimental test (T-history), was created within ANSYS (Figure 1). The model was meshed using a regular quadrilateral mesh, resulting in a finite element mesh comprising 75 elements and 282 nodes. The initial temperature was set based on experimental analysis, with a simulation time of 12 000 seconds and a sub-step duration of 60 seconds. All other calculation mechanism settings were maintained at their pre-set values.

The governing equation in the transient thermal analysis used the model is presented in Equation (1). Where the k is thermal conductivity (W/m K), t is time, T is temperature, q is rate of heat flux, convection, radiation, and internal heat generation inside the volume (W), ρ is density of the material (kg/m^3), c is specific heat capacity of the material (J/kg K):

$$k\nabla^2 T + q = \rho c \frac{\partial T}{\partial t}. \tag{1}$$

The convection value of 3.6 W/m^2 K was set as the boundary condition, which was calculated based on

TABLE 1 Summary of wood material properties used for finite element simulations.

Specimens	Dimensions (mm)	Density (kg/m^3)	Thermal conductivity (W/m K)	Specific heat capacity (J/kg K)
Beech untreated	90 × 9	750.3	0.13	1600[37]
Thermally modified beech (TMB)	90 × 9	656.9	0.10	1450[38]
Untreated beech with BPCM	90 × 9	1038.4	0.2	Varying—based on T-history or DSC
TMB with BPCM	90 × 9	1044.2	0.21	Varying—based on T-history or DSC

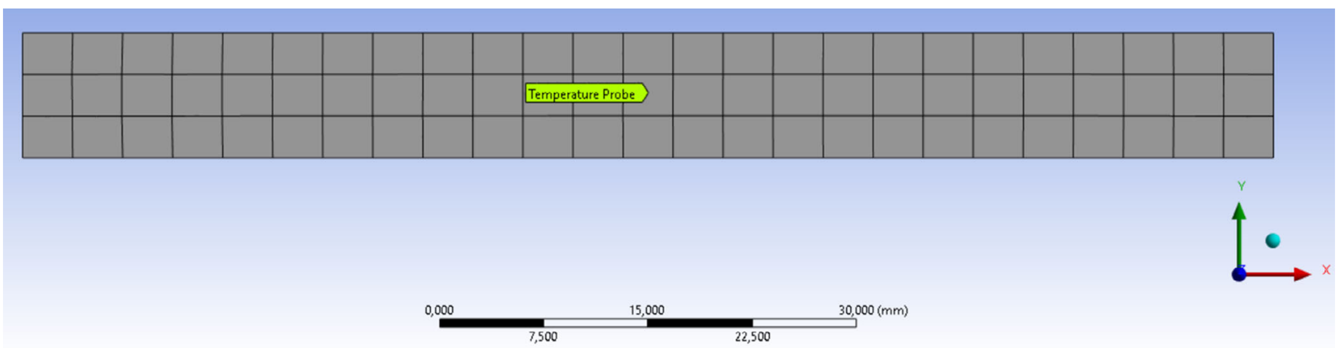

FIGURE 1 Two-dimensional model of the wood specimens in Ansys software with dimensions of 90 × 9 mm.

the thermal resistance of the insulation material surrounding the specimens. Moreover, the cold (0°C) or warm (40°C) ambient temperature were set as ambient air temperature. To input the material properties of specimens impregnated with PCM, particularly the heat capacity in relation to temperature, the specific heat data obtained directly from the T-history and data based on the DSC measurement were used to make the simulation with unadjusted data. To improve the accuracy of the simulations, a novel approach was used, namely, as the latent heat of BPCM-treated wood is known to be proportional to PCM uptake,[27] the specific heat capacity was calculated (Equation 2) as the decrease in the total specific heat capacity of pure PCM as a function of wood uptake.

Equation (2) represents the calculation of the specific heat capacity of the wood composite (wood impregnated with BPCM) over a specified temperature range for heating period. Where the $C_{\text{composite}}(T)$ is the specific heat capacity at a given temperature, $\%C_{\text{pure PCM}}(T)$ is the percentage of the specific heat capacity at a given temperature of the pure BPCM which is incorporated into wood, and $\%C_{\text{wood}}(T)$ is the percentage of the specific heat capacity of the wood present in the composite.

$$C_{\text{composite\_heating}}(T) = \int_b^a \left(\%C_{\text{pure PCM}}(T) + \%C_{\text{wood}}(T)\right). \tag{2}$$

In addition, the freezing temperature was shifted by 2°C to a higher temperature during the cooling phase (Equation 3). The higher freezing point of the BPCM in the wood matrix may be related to the faster nucleation in the microstructure of the wood. Equation (3) shows the calculation for the specific heat capacity of the composite during the cooling period with additional temperature shifting in relation to the DSC measurement. Where the temperature shift of the solidification point is added as T_s.

$$C_{\text{composite\_cooling}}(T) = \int_b^a \Big(\%C_{\text{pure PCM}}(T - T_s) + \%C_{\text{wood}}(T - T_s)\Big). \tag{3}$$

The other simulation parameters, namely density, thermal conductivity, dimensions, boundary conditions, and initial temperatures remained the same as in previous calculations with unadjusted data from DSC and T-History. Although wood is an anisotropic material, which influences, for example, the thermal conductivity, wood was considered as an isotropic material in the simulations to simplify the model.

3 | RESULTS AND DISCUSSION

3.1 | Impregnation process

The results of the impregnation process (Table 2) revealed that the WPG of the specimens was consistently high across all specimens. Notably, the WPG for TMB was higher (54.1%) than that of untreated beech (37.1%). This is likely due to the thermal degradation of cell wall polymers resulting in more cavities where the BPCM can be stored and thus TMB uptakes 22% more BPCM than the untreated beech.

Both specimens achieved a similar maximal level of impregnation, with untreated beech specimens reaching 66.6% and 71.4% for TMB. It is worth noting that beech, particularly its sapwood, is classified as easily treated according to EN350 standard, which is reflected by the high WPG observed in the study. As reported by Nazari et al.[29] and Hartig et al.[28] the factors influencing the absorption of PCM into beech strongly depends on the impregnation parameters and the viscosity of the PCM. While the BPCM easily penetrates the wood during impregnation, it also tends to leach out of the wood once it reaches a liquid state. A simple leakage test was conducted at 40°C for 72 h, which showed that the BPCM is

TABLE 2 Results of the impregnation process and mass loss after a leakage test for the wood specimens.

Specimens	Density (kg/m^3)	WPG (%)	Density after impregnation (kg/m^3)	Retention (kg/m^3)	Maximum possible amount of PCM[a] (kg/m^3)	Achieved impregnation level[b] (%)	Rate of leakage (%)
Beech	759.3 (8.8)	37.1 (1.1)	1077.7 (10.0)	322.3 (7.2)	483.9	66.6	2.5 (0.5)
Beech (TM)	655.4 (9.2)	54.1 (2.1)	1049.4 (5.9)	394.1 (7.9)	551.8	71.4	2.1 (0.9)

Note: SD in parentheses. n = 5.

[a]Theoretical value calculated based on PCM density of 980 kg/m^3 and density of wood cell wall 1500 kg/m^3 according to Hartig et al.[28]

[b]Percentage of impregnation achieved in relation to the calculated maximum amount.

continuously leaching, that is, 2.5% for untreated beech and 2.1% for TMB of loos by the end of the test.

3.2 | Moisture interaction

The EMC of the untreated and TMB specimens measured at three levels of RH and a constant temperature of 23°C are shown in Table 3. TMB exhibits lower moisture uptake due to changes in its chemical composition and degradation of hemicellulose components of wood, particularly a reduction in the number of hydroxyl groups available for moisture adsorption.[39]

The difference in moisture uptake between 50% and 25% RH and 75% and 50% RH are illustrated in Figure 2. The mass increase was calculated by subtracting the mass of the wood before impregnation to exclude the extra mass of BPCM. Between 50% and 25% RH, both untreated beech and beech impregnated with BPCM exhibited a higher increase in moisture uptake compared to TMB with and without BPCM. However, the difference in moisture uptake between specimens with and without BPCM was minimal, indicating that the presence of BPCM did not affect the moisture adsorption behavior of the wood. Between 75% and 50% RH, the specimens impregnated with BPCM absorbed less moisture than their untreated counterparts. This is caused by the high impregnation rate of BPCM, which resulted in less available space for water molecules to accumulate in the wood matrix. Additionally, the medium-long chain fatty acids used as BPCM are hydrophobic and can only interact with a very limited amount of water. It can be inferred that the presence of fatty acids in wood influences its moisture adsorption behavior, particularly in situations where RH is high.

3.3 | T-history

Figure 2 shows the T-history temperature profiles of wood specimens with and without BPCM, and copper plate, during the cooling (Figure 3A) and heating process (Figure 3B). The ambient temperatures were kept constant at 0°C (cold ambient) and 40°C (hot ambient) with ±0.8°C deviation. After being placed in the climate chamber at 0°C, the temperature of specimens with BPCM, and the reference decreased gradually from the initial temperature of 40°C and continued to decrease over time until reaching the cold ambient temperature (0°C).

The phase transition was observed for BPCM during the cooling process, starting at 20°C, but it fully solidified at 21.1°C due to the supercooling effect. The same pattern was observed for beech with BPCM and TMB with BPCM. However, during the heating process, BPCM and specimens with BPCM displayed uniform melting profile at 23°C. Although a slight shift to lower temperatures for wood specimens was observed when compared to pure BPCM.

During the cooling (Figure 3A) and heating (Figure 3B) courses, untreated beech and TMB without BPCM attained temperature equilibrium faster compared to the copper plate and wood specimens containing BPCM. This difference is attributed to the lower thermal capacity of the specimens without BPCM. The temperature profile of the materials in transient conduction condition is directly proportional to the thermal mass of the materials. An increase in thermal capacity by incorporating BPCMs

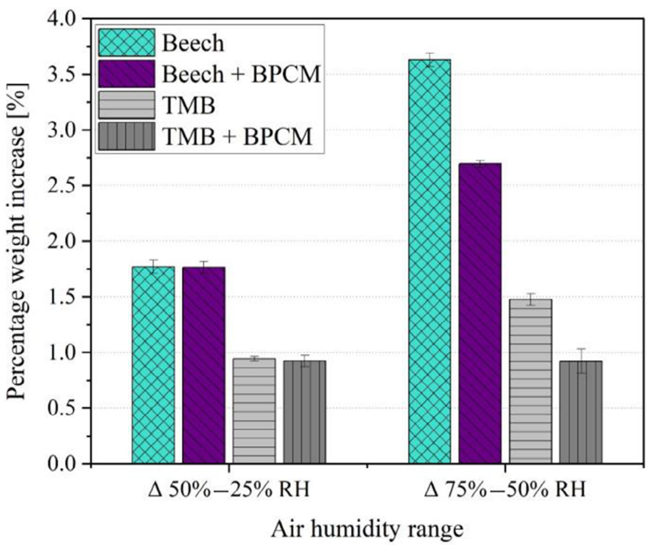

FIGURE 2 Moisture uptake of untreated and impregnated with PCM specimens at two transitions of the RH.

TABLE 3 EMC of the untreated and thermally modified beech specimens at three levels of RH.

	Equilibrium moisture content		
Specimens	23°C/25% RH (%)	23°C/50% RH (%)	23°C/75% RH (%)
Untreated beech	6.0	7.9	11.9
Thermally modified beech	3.2	4.1	5.7

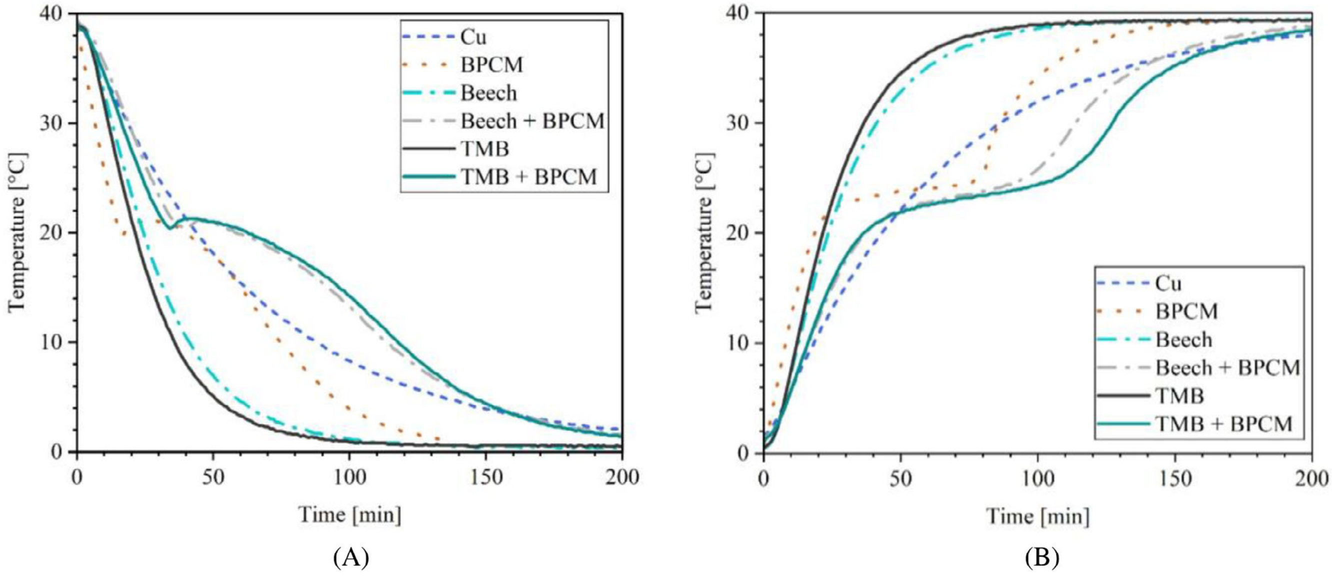

FIGURE 3 T-history temperature measurements inside the specimens with and without BPCM during cooling (A) and heating (B) cycle.

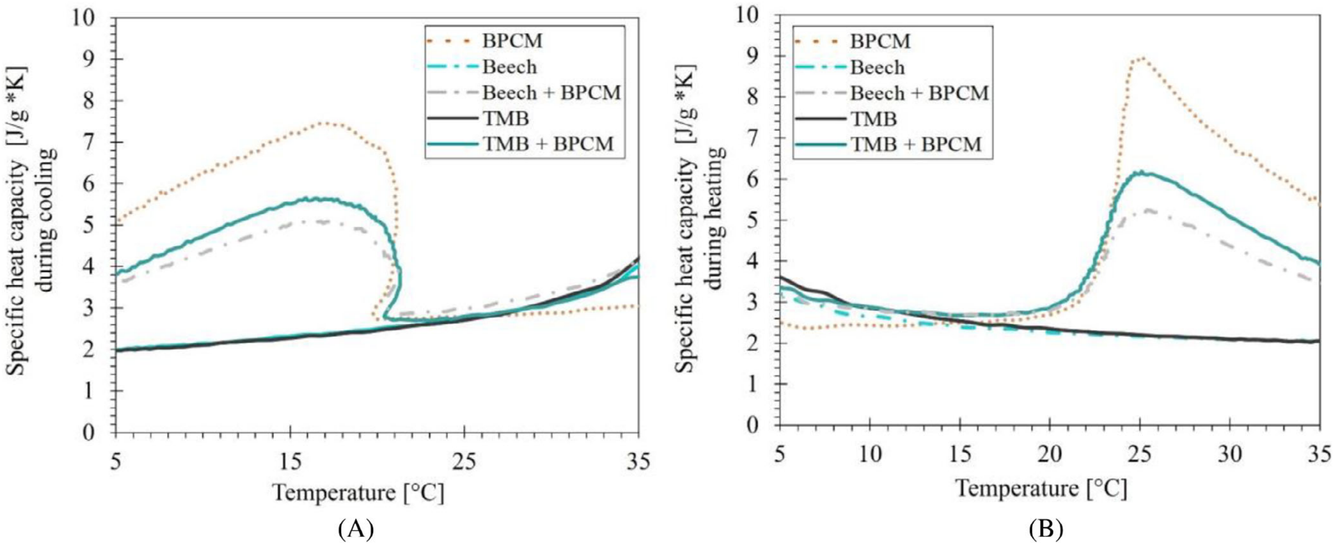

FIGURE 4 Freezing (A) and melting (B) specific heat capacity of wood specimens and pure BPCM calculated based on the T-history measurements.

results in greater energy absorption and storage by the material during heating, and greater energy release during the cooling process, leading to a delay in reaching the ambient temperature.

The incorporation of BPCM into the wood specimens enhances the thermal capacity of the material, allowing it to absorb and store excess energy when the ambient temperatures change (Figure 4A,B). Comparing the untreated beech and TMB, TMB specimens have a lower initial density, and therefore a lower thermal capacity, causing it to attain equilibrium slightly faster than untreated beech. However, the structure of TMB allows impregnate higher amount of BPCM which results in a higher latent heat for TMB.

Figure 5 presents the enthalpy measurements based on the T-history method for the specimens with and without BPCM, as well as for pure BPCM during the cooling and heating courses. The results demonstrate that the specimens without BPCM exhibit a linear pattern that overlaps with findings reported in previous studies,[24,29] indicating that energy is stored and released as sensible heat during the heating and cooling cycles. However, the incorporation of BPCM in the wood specimens enables them to exhibit latent heat storage during phase

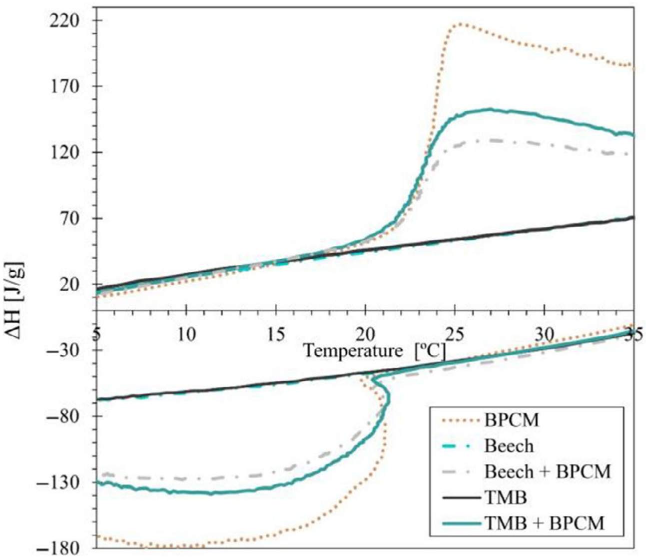

FIGURE 5 Freezing and melting enthalpy of wood specimens and pure PCM calculated based by the T-history measurements.

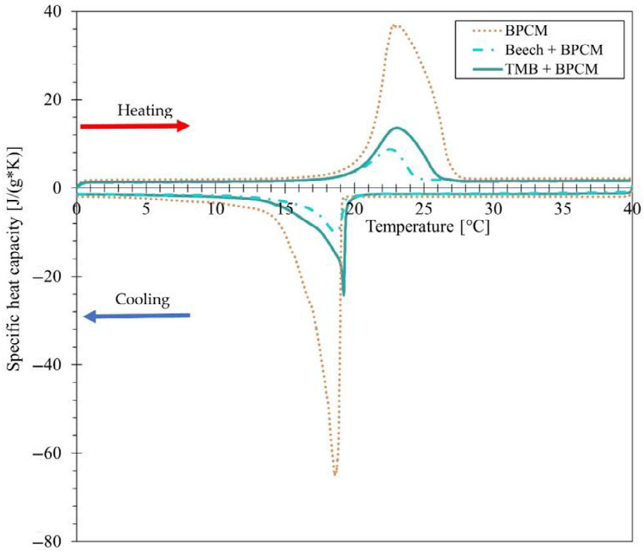

FIGURE 6 Freezing and melting enthalpy of wood specimens impregnated with PCM and pure PCM according to DSC analysis.

transition, while energy is still stored and released as sensible heat before and after phase transition. It is noteworthy that the enthalpy of the specimens with BPCM is dependent on the of BPCM uptake, thus, TMB with higher impregnation uptake exhibits a higher enthalpy than untreated beech with BPCM. The pure BPCM exhibits a latent heat of around 150 J/g during heating and 100 J/g during cooling. The enthalpy of TMB with BPCM during heating and cooling is around 90 J/g and 70 J/g, respectively, whereas the enthalpy of untreated beech with BPCM during heating and cooling is around 75 and 60 J/g, respectively.

3.4 | Differential scanning calorimetry

Figure 6 shows the DSC results indicating the melting temperature of the BPCM at 23.2°C. The melting temperature is observed at 22.4°C for untreated beech impregnated with BPCM, and around 23.1°C for TMB impregnated with BPCM. It is noteworthy that the endset temperature of both impregnated wood specimen is lower than that of pure BPCM. The observed temperature shift of BPCM incorporated into wood determined by DSC analysis and T-history measurement can be attributed to the influence of capillary forces between the BPCM molecules and the cell walls of the wood, which can affect the interfacial interactions and the overall performance of the composite material.[16] Moreover, the visible shift in temperature between these two measurements, namely DSC and T-History, is due to the sensitivity of the instruments and the size of the specimens. The DSC is highly sensitive device and requires small samples (usually 5-40 mg), while the T-History is suitable for measuring bigger samples.

The supercooling effect observed in T-history temperature profiles was not observed in the DSC results, possibly due to the relatively small sample size. Additionally, a comparison of DSC and T-history results revealed that pure BPCM exhibited similar values and temperatures in both methods, except for the supercooling effect.[40] However, it should be noted that the DSC technique, typically optimized for homogeneous materials, yielded discrepant latent heat values for wood specimens infused with PCM. This inconsistency is attributable to the small sample size and high sensitivity of the DSC method, which may inadequately represent the behavior of the composite material. An acknowledgement of this limitation has been made by other researchers, highlighting the need for further investigation into the thermal behavior of BPCM-wood composites using alternative analytical methods with a focus on larger sample sizes.[36]

3.5 | Finite element simulation

The temperature measurements data obtained from T-history analysis were employed to validate the numerical simulations carried out using the FEM. The main objective of the simulations was to identify the optimal approach for determining the thermal properties of the wood specimens, especially the specific heat capacity of the specimens containing BPCM. As it is already known that BPCM incorporated into wood behaves differently than pure BPCM which has been already defined by other researchers as challenging and so far, there is no comprehensive approach for wood impregnated with PCM.[36]

Figure 7 compares the simulations results with experimental data for specimens with and without BPCM. The material properties (specific heat capacity) of simulated specimens were used based on the T-history and DSC analysis for BPCM impregnated specimens. The simulations and experimental data showed high similarity for both cooling and heating courses especially for untreated specimens. For the comparison of the results, mean absolute error (MAE) and root mean squared error (RMSE) were calculated and the results are presented in Table 4. In both cases, the smaller the number, the greater the similarity between the simulation and the experimental data. The comparison of the simulated data to experimental results for untreated beech without PCM resulted in MAE of 0.57°C and 0.6°C for cooling and heating processes, respectively. The TMB without PCM showed similar MAE range of 0.74°C during the cooling period and 0.78°C during the heating period.

Figure 7A–D and Table 4 clearly demonstrate that simulations of specimens without BPCM exhibit greater similarity than simulations of PCM impregnated specimens based on DSC or T-history. Generally, DSC provides a more accurate representation of the material behavior. However, in the case of both beech and TMB, the simulated lines are shifted due to a lower heat capacity in the simulation compared to reality. Additionally, as

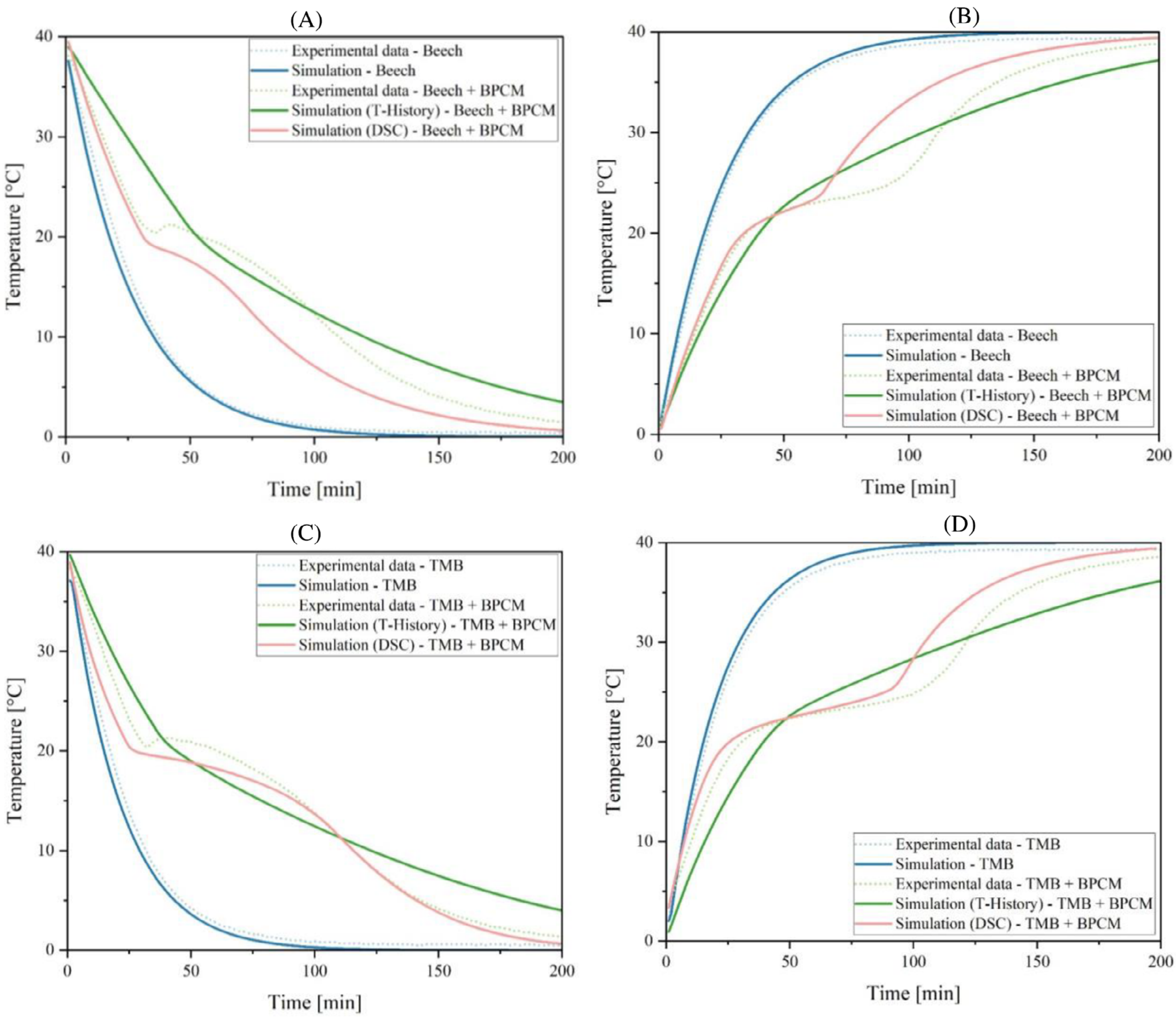

FIGURE 7 Experimental measurement and simulation results of the untreated beech and TMB specimens without and with BPCM; (A) cooling and (B) heating cycle of untreated beech with and without PCM; (C) cooling and (D) heating cycle of thermally modified beech with and without PCM.

TABLE 4 Calculated mean absolute error (MAE) and root mean squared error (RMSE) of the simulated data for beech and TMB with and without BPCM.

		Beech				Beech thermally modified			
		Cooling period		Heating period		Cooling period		Heating period	
Specimens	Source of heat capacity and enthalpy data for simulations	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE
Untreated samples	-	0.57	0.78	0.60	0.63	0.74	0.87	0.78	0.80
Samples impregnated with PCM	DSC	2.63	3.10	1.97	2.90	1.06	1.47	1.65	2.14
	T-history	2.29	2.71	1.87	2.06	2.31	2.49	2.48	2.66
	Calculated[a]	0.60	0.71	0.31	0.40	0.83	1.48	0.70	0.85

[a]Data calculated based on DSC measurement. Description of the calculation in the methodology part.

previously mentioned, the DSC does not reflect the supercooling phenomena, which was prominently observed during the cooling period of the larger specimens during the T-history analysis. Consequently, the simulated data based on DSC indicates a lower melting point. In contrast, simulations based on T-history shows a more linear course with a single kink. Furthermore, the predicted temperature measurements at the end of the experiments deviate from the experimental data and from those observed in DSC-based simulations.

Due to the limited specimen volume used in DSC measurements, the obtained results may not fully represent the behavior of larger wood panels. However, as previously discussed in the study by Nazari et al.,[29] the latent heat of the impregnated wood specimen is directly related to the uptake of the BPCM. Therefore, in order to enhance the similarity between the numerical simulations and experimental data, a novel approach (Equations 2 and 3) was implemented to determine the material properties, namely the specific heat capacity.

Figure 8A,B illustrates the effectiveness of an adjustment, where the latent heat proportional to the PCM uptake was taken into account. This modification led to improved simulations and reduced MAE and RMSE values for the PCM impregnated specimens. The adjustment for the cooling process posed more challenges since the DSC data did not exhibit the supercooling effect observed in the larger specimens. In order to address this, a manual shift of 2°C to higher temperature was applied to the latent heat of the material properties during the cooling process. This modification improved the accuracy of the simulations for both wood specimens, namely untreated beech with BPCM and TMB with BPCM.

However, it is important to note that during the cooling process, the behavior of TMB in liquid state does not accurately reflect the experimental observations. The

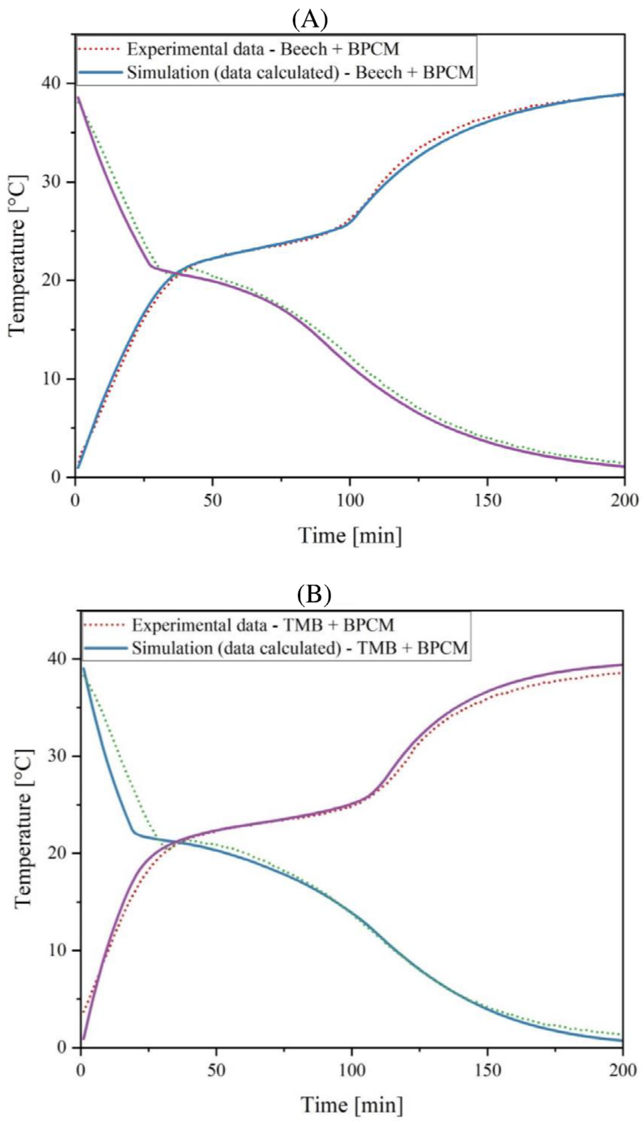

FIGURE 8 Simulations and experimental data for cooling and heating cycle of untreated beech (A) and TMB (B) with PCM utilizing the calculated and adjusted data.

convergence of the lines occurs first when the melting process begins. Consequently, the MAE and RMSE values are relatively high, measuring 0.83 and 1.43, respectively. For the comparison, the beech specimens with BPCM, the MAE and RMSE values are lower, measuring 0.6 and 0.71, respectively.

The results indicate that a combination of both DSC and T-history methods is necessary to accurately model the behavior of BPCM incorporated into wood. DSC analysis is useful for measuring the thermal capacity of homogeneous materials such as pure BPCM, while T-history better captures the interaction of wood and BPCM in bigger specimens, including solidifying temperature and shifts compared to pure BPCM. However, further experiments and validation are needed to refine the approach. Sensitivity analysis might be useful to improve the accuracy of FEM simulations and to define the major influencing factors. Overall, this simple simulation analysis shows the importance of combining different methods and techniques to accurately model the behavior of BPCM in wood, which can have implications for the development of energy-efficient building materials and other applications in the construction industry.

4 | CONCLUSION

The study investigates the use of a ternary mixture of fatty acids (80% capric, 10% stearic, and 10% palmitic) as bio-based phase change material (BPCM) incorporated into beech and TMB. The incorporation of BPCM does not affect the solidification and melting processes, thus the incorporation of this type of materials into wood improves its thermal mass and may contribute to enhancing the thermal efficiency of future buildings without significantly changing the volume of the walls or their weight. The results show that both types of considered wood specimens achieve almost similar level of maximum possible impregnation uptake. However, TMB host approximately 22% more BPCM per cubic meter than untreated beech specimens. TMB with BPCM exhibited a greater rise in latent heat, reaching up to 90 J/g, compared to untreated beech with BPCM, which reached up to 75 J/g. BPCMs incorporated into the wood specimen enhances the thermal mass of the material, allowing it to absorb and store excess energy when the ambient temperatures change. As a result, TMB can hold approximately 70 kg/m^3 more of BPCM than untreated beech with BPCM, and therefore offers a higher thermal mass or lower total volume. However, it is important to note that the use of TMB requires an additional manufacturing step prior to impregnation, which increases the price of the final product. The presence of BPCM in wood structure reduce moisture adsorption behavior, especially in situations where RH is high, the BPCM treated specimens adsorb less moisture.

DSC and T-history analyses presented in this study provided valuable insights into the thermal behavior of BPCM incorporated into beech and TMB specimens. By applying the thermal properties obtained from one of the two analyses, the impregnated wood samples showed a high error between the simulated and experimental values using the FEM. The results showed that a combination of both DSC and T-history methods may be useful to accurately model the behavior of BPCM especially the fatty acid mixture incorporated into wood (beech and TMB) using the FEM. The adjustment, considering latent heat proportional to BPCM uptake and adjustment of the solidifying temperature were necessary to improve simulations and reduced MAE and RMSE for impregnated specimens with BPCM. A reduction of up to 85% in MAE and RMSE was possible, as compared to using single data from either T-history or DSC. However, further experiments and validation is required to refine the approach, with emphasis on improvements to the model (eg, orthotropic), temperature dependency, different boundary conditions, as well as the coupled-thermal-moisture analysis.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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