Modeling Approach to Facilitate Thermal Energy Management in Buildings with Phase Change Materials

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Abstract

This work conceives a numerical modeling approach for the practical application of phase change materials (PCM). Momentum, energy and mass conservation are implemented in a coupled manner including auxiliary algebraic equations for phase change functionality. Key element of the modeling approach is the introduction of a so-called mushy zone at the interface between solid and liquid where the thermophysical properties are smeared out over an user-defined range of melting temperature.
A 2D square cavity test-case shows the influence of natural convection on the melting front propagation. For practical application the model has been adapted to an 1D case representing the wall-crosssection of a typical Norwegian wooden cabin. The model can quickly reveal energetic optimization potential as well as provide orientation among the vast selection of PCM for the target-oriented choice of a suitable material.

Keywords: Phase Change Materials, Natural Convection, Latent Heat Storage Systems, Energy Efficiency in Buildings

1 Introduction

Thermal energy storage systems enjoy increased attention within the framework of worldwide efficiency enhancement efforts. These systems exploit previously captured energy when it is demanded. As such, flexible energy supply applications can be developed leading to an overall efficiency increase of the system. As components of thermal energy storage systems, phase change materials (PCM) are excellent candidates due to their ability to capture and release noticeably large amounts of latent heat during solidification and melting whilst maintaining a constant operating temperature. For building purposes PCM hold great potential to reduce heating and cooling costs (Kuznik et al., 2011) . Further development and optimization by numerical modeling proves to be a powerful tool to navigate through the vast selection and application areas of PCM. In this study, a PCM numerical model for COMSOL Multiphysics® is conceived. Firstly, the theoretical background is elaborated by means of a 2D test-case and subsequently adjusted to the needs of the building industry.

2 Physical Model

The melting and solidification characterstic of PCM pose a true multiphysics problem due to the coupling of fluid flow and heat transfer as illustrated in Fig. 1.

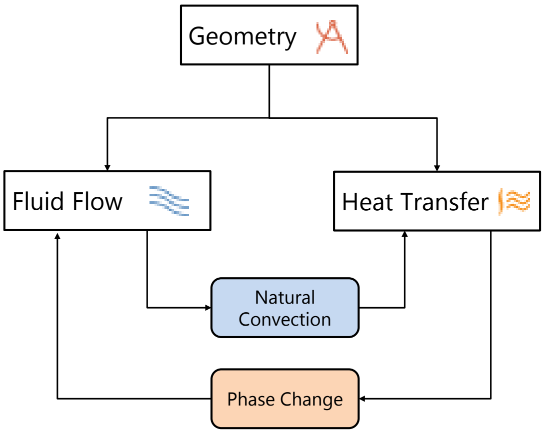

Figure 1. Multiphysics coupling for the solidification and melting processes of PCM.

The coupling is stronger with increasing relevance of natural convection, *i.e.* for sufficiently large temperature differences between boundary temperatures and melting temperature such that bulk forces arise. For boundary temperatures close to the melting temperature the problem might be reduced to the analytically solveable *Stefan* problem respecting heat transfer only (Ogoh and Groulx, 2010).

The chosen 2D test-case geometry is a square cavity as shown in Figure 2. A Dirichlet boundary condition for the temperature ($T_1 = 55°C$) is set at the right-hand vertical boundary while the remaining boundaries are thermally insulated. In the test-case, the paraffin-wax based PCM *n*-eicosane is imposed due to its well-known thermophysical properties as summarized in Table 1.

3 Numerical Model

The distinction between solid and liquid poses a numerical singularity as material properties change rapidly at the melting temperature T_m. To circumvent convergence issues the *enthalpy-porosity formulation* suggests the introduction of a so-called mushy zone where the thermophys-

Table 1. Properties of *n*-eicosane (Muhammad et al., 2015)

	Solid	*Liquid*
density ρ [$\mathrm{kg\,m^{-3}}$]	910	769
thermal conductivity k [$\mathrm{W\,m^{-1}\,K^{-1}}$]	0.423	0.146
heat capacity C_p [$\mathrm{J\,kg^{-1}\,K^{-1}}$]	1926	2400
thermal expansion coefficient β [$\mathrm{K^{-1}}$]	-	8.161×10^{-4}
melting temperature T_m [K]	36.4	-
latent heat / heat of fusion L [$\mathrm{kJ\,kg^{-1}}$]	248	-

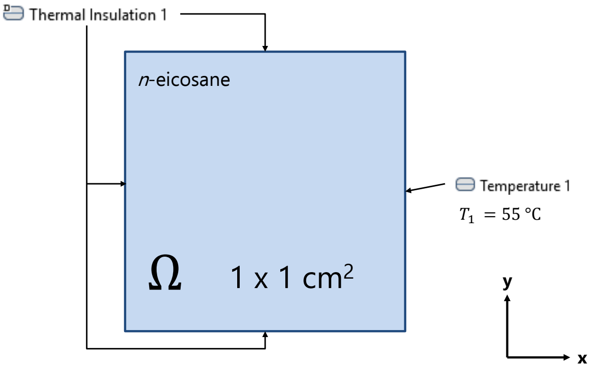

Figure 2. Geometry of the 2D model.

ical properties of the solid and liquid phase are smeared over an user-defined melting temperature range ΔT (Dutil et al., 2011). The main benefit of the porosity formulation is the use of a single mesh to solve the whole set of governing equations for the fluid flow and heat transfer.

COMSOL offers the phase change functionality within the *Heat Transfer Module* (AB, 2017). However, a stable coupling to CFD for buoyant forces requires additional user attention by defining the set of complimentary algebraic equations for material laws.

3.1 Material laws

The melt fraction $\theta(T)$ defines the prevailing state of a material as solid, liquid or mushy zone. The distinction is made upon the current material temperature T as (Kheirabadi and Groulx, 2015; Rubinetti et al., 2018)

$$\theta(T) = \begin{cases} 0, & \text{for } T < T_m - \Delta T/2 \\ \frac{T-(T_m-\Delta T/2)}{\Delta T}, & \text{for } T_m - \Delta T/2 < T < T_m + \Delta T/2 \\ 1, & \text{for } T > T_m + \Delta T/2. \end{cases} \tag{1}$$

Further, in accordance with the energy conservation condition over the user-defined melting temperature range ΔT (here: $\Delta T = 2\mathrm{K}$) the Gaussian distribution function $D(T)$ writes

$$D(T) = \frac{e^{-\frac{(T-T_m)^2}{(\Delta T/4)^2}}}{\sqrt{\pi(\Delta T/4)^2}}. \tag{2}$$

Equations (1) and (2) are implemented into a customized expression for the temperature-dependent heat capacity $C_p(T)$ as

$$C_p(T) = C_{p,s} + \theta(T)(C_{p,l} - C_{p,s}) + D(T)L. \tag{3}$$

Similarly, expressions for the thermal conductivity and density are obtained, without the $D(T)$ term. The set of equations can conveniently be implemented in COMSOL as analytical expressions. Lastly, the correlation for the viscosity as a function of temperature for *n*-eicosane is given by:

$$\mu_l = (9 \times 10^{-4} T^2 - 0.6529T + 119.94) \times 10^{-3}. \tag{4}$$

3.2 Physics

Within the tool, two physics are needed to ensure a complete PCM model for the 2D test-case,

Laminar Flow Assuming incompressibility and neglecting inertial terms. The Boussinesq approximation has proven suitable for PCM modeling which is activated by including gravity and using reduced pressure.

Heat Transfer in Fluids In the fluid definition the primarily defined analytical expressions for the material laws are to be inserted.

The CFD part of the study requires an additional modeling term $S(T) \cdot \boldsymbol{u}$ in the governing equations accounting for the porosity of the mushy zone. The porosity function $S(T)$ is derived from the Carman-Kozeny equation writing

$$S(T) = A_m \frac{(1-\theta(T))^2}{\theta(T)^3 + \varepsilon}. \tag{5}$$

The mushy zone constant A_m has been reported to perform most accurately for a value of 10^6 $\mathrm{kg\,m^{-3}\,s^{-1}}$ (Kheirabadi and Groulx, 2015). The constant ε is solely needed to avoid division by zero. As such, the value can be set small, *e.g.* to 10^{-4}.

3.3 Mesh

The square geometry allows for an uniform mapped mesh. As reasonable trade-off between accuracy and computational time a distribution of 100×100 cells is used in the 2D test-case according to findings in another work (Rubinetti et al., 2018).

4 Test-case results

The results of this test-case show the suitability of the COMSOL model to capture convective effects as illustrated by Figure 3.

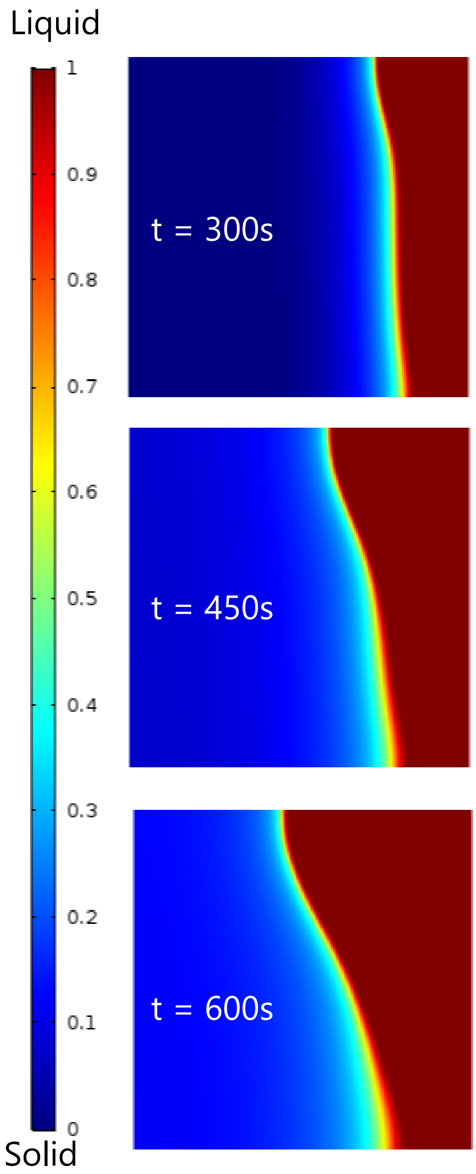

Figure 3. Melting front location during the transient melting process of the 2D test-case - color scale according to the melted fraction $\theta(T)$.

5 Application example

This section includes the analysis conducted by (Rubinetti, 2018) to demonstrate the practical aspect of PCM modeling. A successful use of PCM for building purposes should take the type of PCM, the construction of the building and the climate into consideration (Pasupathy et al., 2008). The numerical model is adapted to a 1D case representing a wall cross-section, thus switching from material-level to room-level. Unidirectional heat transfer by conduction is a popular assumption for a preliminary assessment in numerical studies of buildings (Kuznik et al., 2011). As a local phenomenon, natural convection within the PCM is assumed to be irrelevant for the qualitative performance at room-level. Other convective and near-wall effects are also neglected.

5.1 Physical and numerical model setup

As an example for the physical model a typical scandinavian cabin is considered in accordance with regulatories issued by Norwegian building authorities (TEK 17, 2017). The wall-crosssection of such a building consists of various layers as represented by Figure 4. The physical properties of the various layers are listed in Table 2. Between the encladded non-structural soft wood $\boxed{2}$ and the structural CLT wood $\boxed{4}$ a PCM layer $\boxed{3}$ is implemented. The material is a commercially available PCM called bioPCM $^{\text{TM}}$ (bio).

Table 2. Physical properties of the wall crosssection layers according to figure 4 at reference temperature $T_{ref} = 25$ °C and PCM properties for solid (s) and liquid (l) state

Layer	Width [mm]	ρ [kg m^{-3}]	C_p [J kg^{-1} K^{-1}]	k [W m^{-1} K^{-1}]
$\boxed{1}$ $\boxed{7}$	50	1.3	1000	0.13
$\boxed{2}$ $\boxed{6}$	15	390	1600	0.13
$\boxed{3}$ (s)	9	1400	2200	2.5
$\boxed{3}$ (l)	9	850	4500	0.15
$\boxed{4}$	100	410	1300	0.098
$\boxed{5}$	120	60	850	0.04

The chosen PCM has a freezing point of 18.5 °C and a melting point of 23 °C meaning that there is a temperature margin where both phases can co-exist. This effect is known as thermal hysteresis which has to be included in the model. An additional ordinary differential equation has to be solved alongside the *Heat Transfer in Fluids* interface to account for the current phase state. With the newly defined variable the heat capacity, thermal conductivity and density can be modified with the logical operator `if(condition,expression1,expression2)`. A detailed step-by-step guide on including thermal hysteresis in phase change processes in COMSOL is presented by (Frei, 2016).

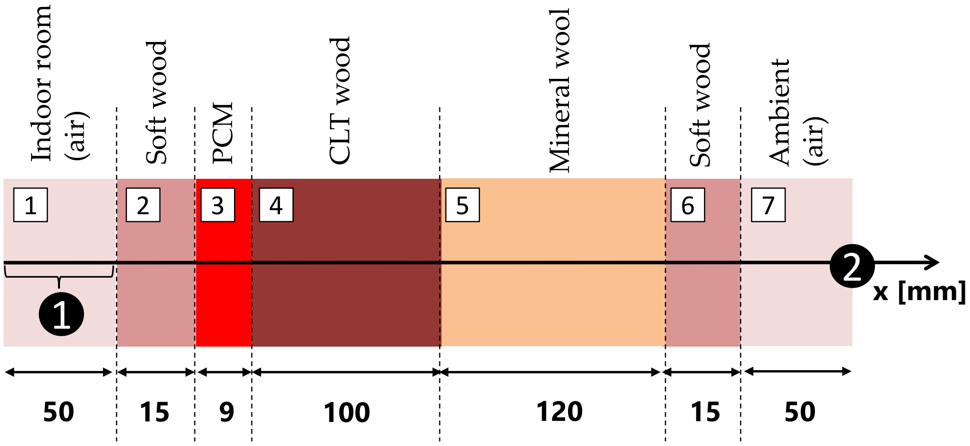

Figure 4. Sketch of a Norwegian cabin wall crosssection with a bioPCM^{TM}layer (bio).

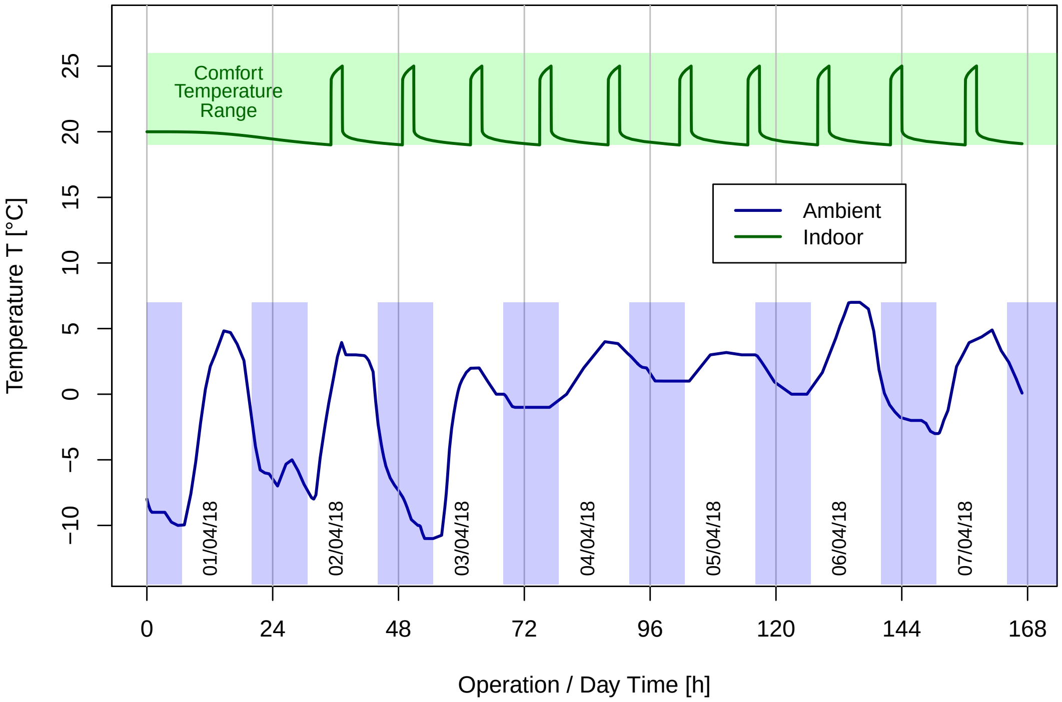

Figure 5. Indoor and ambient temperature curves for Oslo from the 1st to the 7th of April (wea, 2018) for a wall with PCM. The room temperature regulation kicks in on 2nd of April and continues uniformly for the rest of the week.

Further adjustments and definitions of the application example model are listed as follows

- Indoor temperature kept at $T = 21$ °C → Dirichlet BC ①
- Outdoor temperature determined by weather data of Oslo for 1st to 7th of April 2018 (wea, 2018), see Figure 5 → time-dependent Dirichlet BC ②
- Respecting internal heat sources such as people, lighting, electrical equipment as internal heat gains and radiation from weather data (Komité-SN/K-034, 2016; wea, 2018), Fig. 6 → contribute to BC ①
- $\Delta T = 0.01$ K
- Mesh resolution of 10 elements per mm

The simulation runs from $t = 0$ s to 604800 s (1 week) with a writing interval of 500 s which takes 7 minutes of CPU time on a high-performance cluster.

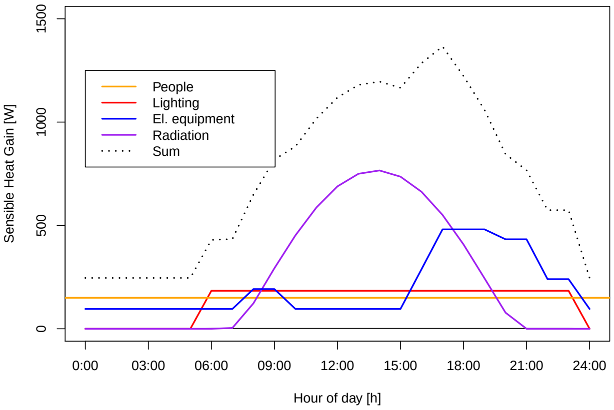

Figure 6. Reference internal heat gains in building applications over a day in April (Komité-SN/K-034, 2016).

5.2 Results and discussion

The PCM can release its stored latent heat to reduce heating demand in the building. The normalized curves in Figure 7 indicate the heater workload savings, *i.e.* the time when the heater is **idle**. It turns out that during the observed April 2018 week the heater is idle approximately half of the time with the PCM increasing the savings marginally by $\sim 1.54\%$.

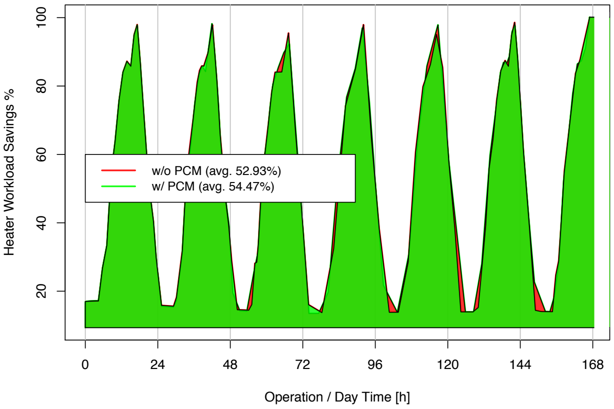

Figure 7. Heater workload savings when maintaining an average indoor temperature of $T = 21$°C. Over the course of the week it can be observed that using a PCM is capable of increasing savings of external energy by $\sim 1.54\%$.

Obviously, over the course of the observed week the energy efficiency does not improve enough to justify increased building costs. In general, it has been proven that PCM can contribute more to the reduction of cooling demand during summer than the reduction of heating demand during winter. Nevertheless, the use of a PCM reduces peak temperatures on both extremes. In a cold climate as in Norway with respect to other building parameters, however, the impact of PCM is expected to be more significant in handling temperatures above 26 °C (Madessa, 2014).

In a hypothetical case where the wall contains no insulation other than the CLT wood and PCM layer and the indoor temperature is kept between 19 °C and 26 °C with a thermostat functionality (Frei, 2015) the benefit of using PCM can be illustrated distinctively. Figure 8 represents the operation times and duration of the room heating facility. It can be observed that the latent heat of the PCM effectively reduces heating demand for a scarsely insulated wall during the observed week of April. Figure 5 compares the internal temperature controlled by the thermostat and the external temperature.

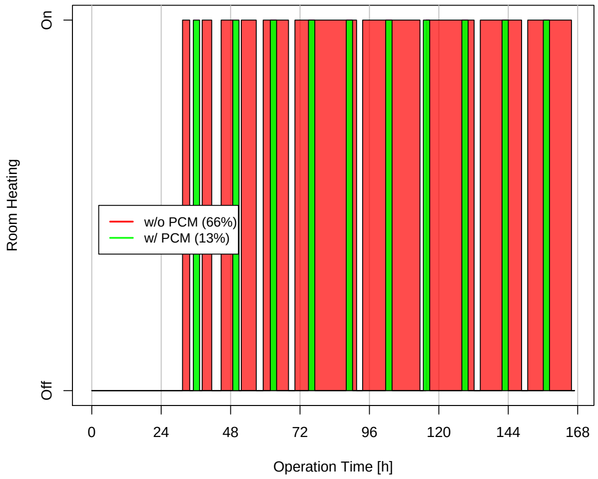

Figure 8. Graphical representation of the thermostat operation time during the week. The overlap between the case with and without PCM shows clearly the increased energy demand of the non-PCM simulation to maintain a comfortable indoor temperature.

The influence of the PCM on the inner wall surface temperature is shown in Figure 9 alongside with the current phase state. In this simple 1D example the vast optimization potential becomes apparent due to the large number of optimization variables. Straightforward and reverse engineering can be conducted with the model, *i.e.* choose a PCM and observe its performance under various set of indoor dynamics or adjust the external requirements to find a suitable PCM both for energy performance and thermal comfort. The power of the 1D model is that results can quickly be obtained and compared, thus, significantly accelerating PCM design work.

6 Conclusion

In this study, a comprehensive modeling approach for phase change phenomena has been developed. The

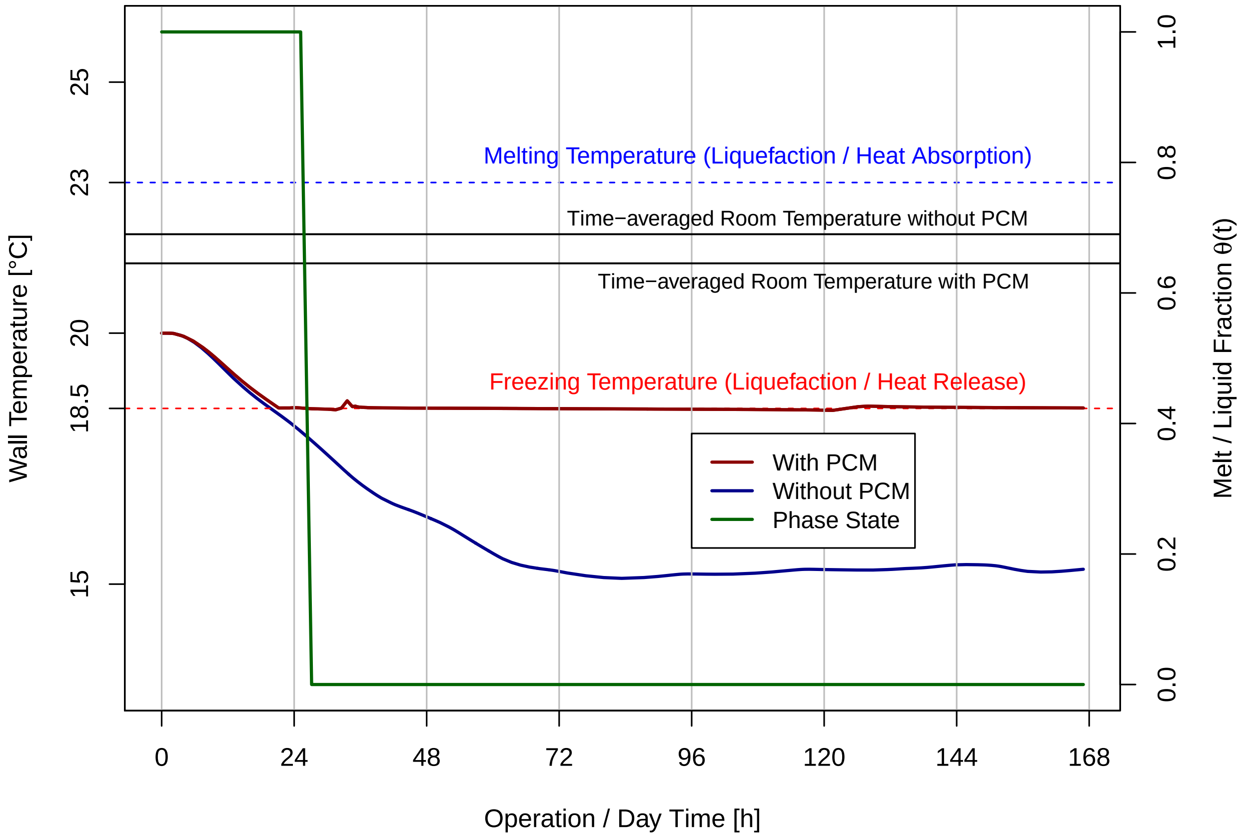

Figure 9. Temperatures measured inside the PCM layer for the hypothetical wall cross-section without additional insulation layers other than the CLT wood and PCM. As expected, the PCM layer maintains its constant temperature after reaching the freezing point while the simulation without PCM indicates a stronger decay of temperature.

enthalpy-porosity formulation proves to be a powerful technique to solve momentum, continuity and energy-equation on the same stationary grid while constraining the natural convection only in the fluid region. The porosity assumption of the mushy zone is a reasonable trade-off between physical accuracy and CPU resources needed. The model can be used to (i) observe in detail the material melting and solidification process, *e.g.* to improve the amount of molten fraction by varying the 2D geometry and (ii) as 1D model for a rapid orientation whether the PCM meets thermal, technical and economic requirements for applications, *e.g.* for a preliminary estimation of energy savings in buildings with PCM layers in external walls.

Furthermore, the 1D case shows the importance of including indoor dynamics - such as internal heat gains and radiation - in the model to assess the PCM potential. Only in interaction with indoor and outdoor conditions the conductive heat transfer through walls delivers insight into the optimal criteria for a PCM candidate with the right latent heat and melting point.

The 2D model as well as the 1D model are numerically stable and suitable for advanced PCM analyses, *i.e.* for the promising future of enhanced PCM (Fleischer, 2015).

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