# FINITE ELEMENT MODELING FOR SOLID-SOLID PHASE CHANGE MATERIALS WITH VARYING HEATING AND COOLING PHASE CHANGE TEMPERATURES

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## ABSTRACT

Phase change materials (PCMs) can be implemented into building practice to enhance thermal storage performance, reduce indoor temperature fluctuations and improve the comfort of occupants. Solid-solid PCMs (SSPCMs) have unique properties which make them superior to the traditional solid-liquid PCMs (SLPCMs). These include an enhanced structural integrity and ease of incorporation with building fabrics. In order to investigate any new type of SSPCM, it is desirable to have a finite element model (FEM) for the thermal performance validated by the experimental data. Due to the impurity and thermal instability, practical PCMs usually do not have the same phase change temperatures on heating and cooling processes. This varying thermal property will affect the validation of FEM, if it is not properly represented. In current study, a mathematical model for SSPCMs will be described and a corresponding FEM will be created in FEMLAB. A script was written for the FEMLAB solver to alter the phase change temperature automatically based on the heating and cooling mode. The enthalpy method and effective heat capacity method were used for the simulation.

## INTRODUCTION

Building energy consumption and its resulting greenhouse gas emissions can be substantially reduced if solar energy is adequately utilized. Storage of thermal energy in buildings has gained prominence in the past two decades due to a strong need to reduce the total thermal energy requirement (both heating and cooling) in buildings (Zalba *et al.*, 2003). The integration of phase change materials into building fabrics can accumulate the gain from solar radiation during the day and release the stored energy at night. Therefore, the energy requirement at peak hours can be reduced and pre-cooling or heating becomes possible. Furthermore, the implementation of PCMs can reduce the indoor temperature fluctuations and improve the thermal comfort of occupants.

The most popular type of PCMs available currently is of the solid-liquid type, which includes two major groups, organic and inorganic compounds (Trp, 2005). Organic compounds exhibit various advantages such as being non corrosive, having low or no supercooling, chemical and thermal stability, and compatibility with conventional building materials. However, they encounter several disadvantages like low phase change enthalpy, low thermal conductivity and flammability. Inorganic compounds present a greater phase change enthalpy, usually twice the value of organic compounds, and also possess high thermal conductivity. The main disadvantages of inorganic compounds are corrosion, supercooling and lack of thermal stability.

Despite their high energy storage density and other advantages, most currently available PCMs suffer from inefficient energy recovery and reduction in overall thermal performance during the solid-liquid phase transition (Farid *et al.*, 2004). Considering the ever-increasing application of PCMs in building practice, PCMs in the liquid state affect the structural integrity and cause undesirable “wetness” in the walls. The aforementioned difficulties could be avoided if SSPCMs are employed.

Practical PCMs also exhibit different phase change temperatures on heating and cooling processes due to their impurity and thermal instability. Paraffin wax, for instance, melts and solidifies in the range of 30-40 °C and 50-60 °C, respectively (Bentz and Turpin, 2007).

In order to mathematically understand the heat transfer phenomenon during solid-solid phase transition, a brief review of the numerical methods of thermal performance of the solid-liquid PCMs is helpful and necessary. During the solid-liquid phase transition process, heat transfer at the moving solid-liquid interface becomes a transient, non-linear phenomenon, which is often called the “moving boundary” problem (Alexiades and Solomon, 1993). The existence of the non-linear convective term in the liquid phase requires the solution of partial differential equations, thus making the moving boundary problems difficult to solve (Myers, 1971).

The finite difference method or finite element method are often used to solve phase change problems. The most common numerical methods are the enthalpy method and the effective heat capacity method. These methods allow a wide range of phase transition temperature of PCMs (Lamberg *et al.*, 2004).

Lamberg *et al.* (2004) carried out finite element analysis on the technical grade paraffin with FEMLAB, and indicated that the effective heat capacity method, when used with a narrow temperature range, gave the closest prediction when compared with the experimental data. However, the phase change temperatures used for the simulation are the same for heating and cooling processes, which was not suggested from the differential scanning calorimetry (DSC) curve. For the application of PCMs in building practice, the characteristic of different phase change temperatures on heating and cooling is especially important since it determines at what degree the energy is stored and released. The proper modeling on the phase change temperature will help to understand the effectiveness of PCMs on the energy performance in buildings.

Zhang *et al.* (2007) studied the thermal performance of a concrete compound integrated with a hypothetical SSPCM of varying PCM concentration and thickness. The finite element analysis on FEMLAB indicated that the overall thermal behavior of the compound is subject to not only the thermal capacity of PCMs, but also the thermal resistance of the compound. However, the difference in phase change temperatures on the heating and cooling processes were not taken into consideration in the study.

## OBJECTIVE

The objective of this study is to modify the previous FEM (Zhang *et al.*, 2007), and to analyze the impact of different heating and cooling phase change temperatures in the FEM. A script will be written in the solver to achieve the automatic alteration in thermal properties depending on the heating and cooling mode. The new FEM will be used as a tool for the future experimental validation.

## NUMERICAL METHODS

The governing equations for the heat transfer process in the solid-liquid PCMs are composed of the Navier-Stokes (momentum) equations, the mass conservation equation, and the energy conservation equation. From a mathematical point of view, the momentum and mass conservation equations can be neglected for the solid-solid PCMs because there is no convective term in the PCMs. This conclusion significantly simplifies the numerical analysis. Therefore, the energy equation is the only governing equation for the analysis of SSPCMs, and can be expressed as follows,

$$\rho C_p\left(\frac{\partial T}{\partial t}\right)=\nabla(k\nabla T) \qquad (1)$$

where $\rho$, $C_p$ and $k$ are the density, specific heat and thermal conductivity of PCMs, respectively.

Upon heating or cooling, sensible and latent heat pass through the PCM simultaneously and the phase transition does not occur uniformly in the PCM. Furthermore, the phase transition usually happens in a non-isothermal temperature range. In case of a solid-liquid PCMs, it is nearly impossible to track the solid-liquid interface, thus making the heat transfer calculation difficult. Therefore, it is desirable to solve the PCM problem in a whole constrained domain (Lamberg *et al.*, 2004). There are two types of numerical methods often used to solve the PCM problems, namely enthalpy method and effective heat capacity method.

The enthalpy method enables the governing equations to be applied over the entire domain of interest rather than on the phase change interface. The total energy required for the phase change, i.e. the overall sensible heat and latent heat, can be determined by the enthalpy function $H(T)$. For the SSPCM, the enthalpy term for the energy equation (Eq.1) can be expressed as follows

$$\rho\frac{\partial H(T)}{\partial t}=\nabla(k\nabla T) \qquad (2)$$

An alternate way of solving the non-isothermal phase transition in PCM is the effective heat capacity method. The effective heat capacity of the material ($C_{eff}$) is a linear function of the latent heat of fusion on both the heating and cooling processes. It is inversely proportional to the temperature difference between the onset and the end of the phase transition (Peippo et al., 1991). The effective heat capacity of the PCM during the phase change is given as,

$$C_{eff}=\frac{L}{T_e-T_o}+C_p \qquad (3)$$

where $L$ is the latent heat of fusion, $T_o$ is the onset temperature of phase transition happens and $T_e$ is the temperature when the phase transition completely finishes. Thus, the governing equation (Eq.1) for the binary solid state PCM can be expressed as

$$\rho C_p(T)\left(\frac{\partial T}{\partial t}\right)=\nabla(k\nabla T) \qquad (4)$$

$$C_p = \begin{cases} C_p & T < T_o \\ \dfrac{L}{T_e - T_o} + C_p & T_o \le T \le T_e \\ C_p & T > T_e \end{cases} \quad (5)$$

## SIMULATION

The simulations were carried out in FEMLAB. A piece of hypothetical SSPCM with 20 mm in thickness was modeled, as shown in Figure 1. The PCM was subjected to a constant heat flux of ±300 W/m$^2$ over the upper surface, with all the other boundaries thermally insulated. Four measurement points were located in equal intervals in the model to track the temperature variations.

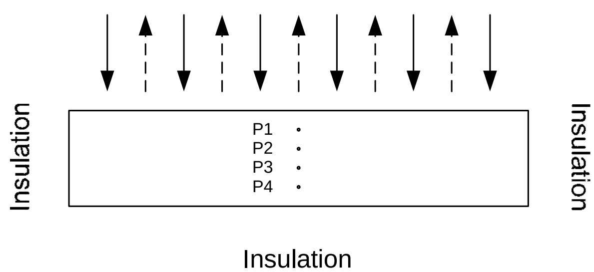


*Figure 1 PCM modeling*

The thermo-physical properties of the hypothetical PCM are presented in Table 1. In order to investigate the effect of varying heating and cooling phase change temperature on the thermal performance, two scenarios were applied over the domain. The first scenario assumes the phase transition occurs in the same temperature range between 22 and 23 °C on heating and cooling. The second scenario assumes a phase change temperature between 22 and 23 °C on heating and between 18 and 19 °C on cooling. The latent heat remains the same as before, at 90 J/g on heating and cooling for both cases.

Other assumptions made in the simulation are given as follows,

1. The density and the thermal conductivity of the compound are constant.
2. The heat transfer across the compound is considered as one-dimensional.

*Table 1 Thermo-physical properties of the PCM*

| **Property** | | **Value** |
|---|---|---|
| Density ($\rho$) kg·m$^{-3}$ | | 800 |
| Thermal conductivity ($k$) W·m$^{-1}$K$^{-1}$ | | 0.3 |
| Specific heat ($C_p$) J·g$^{-1}$K$^{-1}$ | | 1.6 |
| Phase change temperature °C Case 1 | heating cooling | 22/23 |
| Phase change temperature °C Case 2 | heating | 22/23 |
| | cooling | 18/19 |
| Latent heat of fusion ($L$), J·kg$^{-1}$, | | 90000 |

Since the enthalpy method requires the interpolation from the actual DSC curve, which is not applicable to the hypothetical material, this method will not be used in current study. The effective heat capacity method is the only method applied for the simulation. On the heating mode, a constant heat flux of 300 W/m$^2$ was applied for 4500 seconds, followed by the cooling mode with the same amount of heat flux but in opposite direction for another 4500 seconds. A solver script was written to help to solve the heating and cooling modes continuously. The script shows its advantages for multiple thermal cycling runs.

As indicated by Zhang *et al.* (2007), the temperature cannot be distributed homogenously through the PCM slab during the heating and cooling processes, due to the large thermal resistance. Hence, a comparably small "homogenous" domain is adopted to validate the model, before it is extended to the PCM slab. The homogenous domain has a spherical shape with 2mm in diameter. The aforementioned material properties were used and the constant heat flux with the value of 20 W/m$^2$ was applied.

## RESULTS AND ANALYSIS

The first step of the work was to ensure that the model could represent the phase change process, i.e., the temperature vs. time profile should clearly show the different slopes within the phase change temperature range. A constant heat flux boundary condition was chosen to help demonstrate this difference, although it is hard to achieve for the cooling process in practice.

Figure 2 shows the temperature variation in the heating mode in the homogenous domain. The temperature profile represents any point in the domain. As can be seen, the curve departs distinctly at the phase change temperatures between 22 and 23 °C, respectively. The smaller slope in between indicates the energy storage during the phase transition.

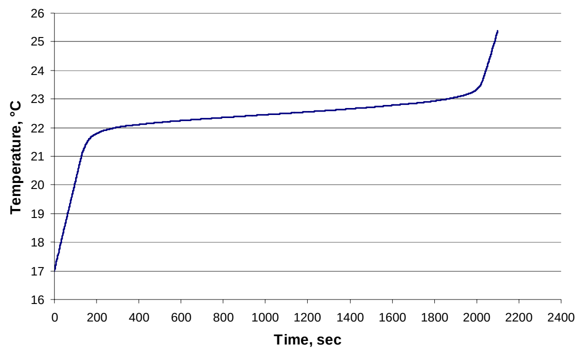


*Figure 2 Temperature profile in the heating mode in the homogenous domain*

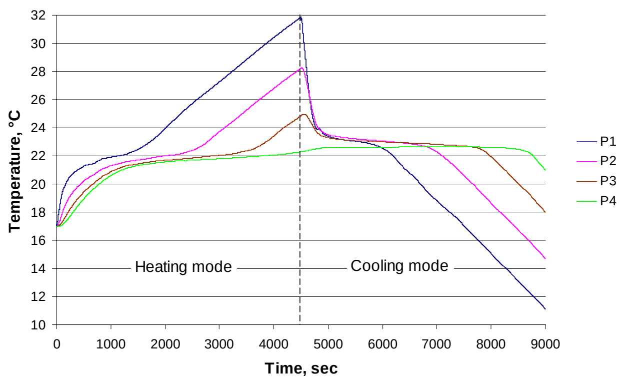


*Figure 3 Temperature profile in the PCM for one heating and cooling cycle, $T_{pc}$ = 22-23°C, Case 1*

Figure 3 shows the temperature profile of the four measurement points in the PCM slab for one heating and cooling cycle. The phase change temperatures are the same for both the heating and cooling modes, as indicated in Case 1. As can be seen, phase transition occurs in sequence from P1 to P4 in the heating mode, with an increase in the duration of phase transition. The thermal energy passes through the PCM as the sensible heat and latent heat. The temperature profile suggests that the latent heat dominates and is stored in the portion closest to the heat source before any sensible heat passes through. The latent heat is stored in the PCM, portion by portion, resulting in a time lag between each point. In the cooling mode, the temperature drops quickly and the phase transition occurs almost simultaneously in P1-P3. This can be attributed to the fact that sensible heat dominates until P1-P3 reaches the onset of phase transition. It is interesting to notice that the phase change temperature in the cooling mode is slightly higher than that in the heating mode, although the setting is the same in the simulation. This could be attributed to the intensive sensible heat transfer that causes the phase transition. The continuous increase in temperature at P4 during the cooling process is because the stored energy in the PCM is transferred to the lower portion, in addition to the surroundings.

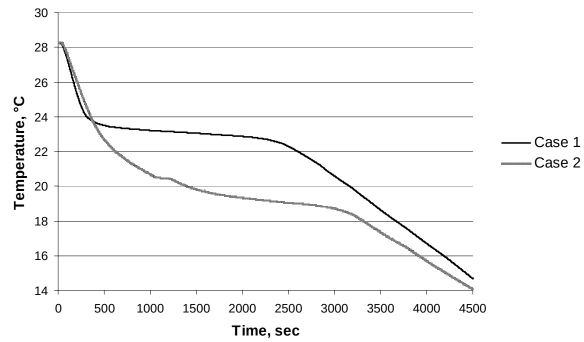


*Figure 4 Temperature profile at P2 in the cooling mode*

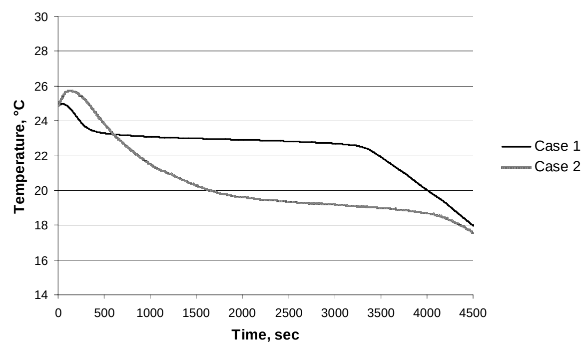


*Figure 5 Temperature profile at P3 in the cooling mode*

The comparison of the temperature profiles between Case 1 and 2 at P2 and P3 in the cooling mode are shown in Figures 4 and 5, respectively. As can be seen, the phase transition in Case 2 occurs in the predicted temperature range (18-19°C). The lower phase change temperature results in the lower temperature level. This characteristic is very important in building practice, since it helps designers choose the proper PCM to use in different regions. In the regions where the average temperature is high, PCMs with lower cooling phase change temperatures are suggested since they can retain a comfortable temperature level for a longer time in the evening. In cold regions, such as Canada, PCMs with higher cooling phase change temperatures are suggested since the temperature can remain at a higher level in the evening.

## CONCLUSIONS

A finite element model was developed for SSPCMs with varying heating and cooling phase change temperatures. Thermal performance of the PCM was analyzed under the condition of a constant heat flux. The temperature profile clearly demonstrates a small slope during phase transition range. The simulation results suggest that for certain PCMs with a given amount of latent heat, different phase change temperature will provide different levels of indoor temperatures, thus affecting the level of indoor comfort of the building.

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