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An Effective Thermal Conductivity-based Approach for Modelling of Convective Heat Transfer in a Rectangular Cavity Filled with PCM

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This paper presents a numerical modelling approach to investigate convective heat transfer in a rectangular cavity filled with a Phase Change Material (PCM), specifically organic paraffin-based Rubitherm RT 35 HC. Natural convection occurs during both the melting and solidification processes due to the changes in the density of a liquid PCM. Therefore, a significant enhancement of the heat transfer in the upper part of the cavity can be observed. The study aims to investigate, both experimentally and numerically, the effect of convective flow on the overall heat transfer performance of a PCM in the cavity. The computational analysis was performed using a two-dimensional explicit finite difference model implemented in MATLAB. To accurately represent the thermal behaviour of the PCM enclosed in a cavity, the proposed modelling approach incorporates the effects of natural convection by considering the effective thermal conductivity of the PCM as a function of both temperature and position within the cavity. By doing so, heat transfer in the upper part of the cavity is enhanced while heat transfer in the bottom part is mitigated, resulting in a more precise representation of the actual thermal behaviour of the PCM. The comparison between the constant thermal conductivity and the effective thermal conductivity with a linear increase has been made, resulting in a significant improvement in the model accuracy. The analysis demonstrated that the effective thermal conductivity approach led to a significant improvement in the accuracy of the numerical model. Specifically, a reduction of 47.5 % was observed in the root mean square error (RMSE) value, decreasing from 4.0 K to 1.9 K.

1. Introduction

Phase Change Materials (PCMs) have been extensively investigated due to their potential for thermal energy storage (TES) in various applications. They offer several advantages over traditional sensible heat TES materials, such as high thermal storage capacity, high energy density and their ability to maintain a nearly constant temperature during the phase change process (Liao et al., 2018). TES systems employing PCMs are also usually very low maintenance with cheap operational costs. These properties make PCMs an attractive option for a wide range of applications, including solar energy storage, building insulation, temperature stabilisation, electronic cooling or as a potential solution for thermal management in the food industry (Ismail et al., 2022). In addition, PCMs are also environmentally friendly and sustainable (Peng et al., 2020), which makes them a promising option for reducing the carbon footprint of various energy systems. In general, PCMs are well capable of withstanding numerous heating and cooling cycles without any significant degradation, making them a very thermally stable option. The use of PCMs can help to improve the overall energy efficiency of a system, as they can store and release thermal energy more efficiently than other storage materials.
Despite the advantages of PCMs, there are still some challenges that need to be addressed. In most cases, numerical simulations of TES with PCMs are based only on heat conduction models, as heat conduction is very often the main contributing factor to heat transfer in PCMs. This is mainly due to the fact that researchers very often construct experimental measurements in a way which mitigates the effects of natural convection. This is typically accomplished by reducing the dimensions of the cavity (height, thickness) and employing a slower heating/cooling rate (Thonon et al., 2021). Another approach to circumvent natural convection is the utilisation

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of composite materials, such as cement mortar infused with varying quantities of microencapsulated PCM (Zalewski et al., 2019). Additionally, altering the heating/cooling direction, such as heating from the upper surface, has been found to mitigate the impact of natural convection (Cheng et al., 2013). However, when a larger volume of PCM is investigated, natural convection in the liquid PCM also becomes a significant contributor to the overall heat transfer process (Amin et al., 2014). Specifically considering heat transfer in the vertical rectangular cavity filled with a PCM, numerical simulations have shown that the heat transfer process is strongly influenced by the convective flow patterns, which develop within the liquid phase of the PCM, as illustrated in Figure 1. More complex modelling techniques that incorporate both heat transfer modes are required to accurately predict the performance of PCM-based systems.

In recent years, many authors investigated the possible utilisation of effective thermal conductivity to solve heat transfer problems experiencing natural convection. A study conducted by (Amin et al., 2014) involved ANSYS simulations to analyse three-dimensional spherical capsules. A simplified modelling approach was employed to investigate heat transfer in PCMs enclosed within spherical capsules. This approach became more feasible when an effective thermal conductivity was determined to represent the natural convection phenomenon occurring within the PCMs. Similarly, the constrained melting process of a PCM in spherical encapsulation was investigated by (Liao et al., 2018). The simulations were conducted using a validated numerical model that included natural convection. The study found a significant difference in the changes in liquid fraction obtained from the model considering natural convection and the conduction-controlled model with thermal conductivity correlations. As a result, the authors proposed a novel correlation for effective thermal conductivity based on the simulation results of the models containing natural convection. The proposed correlation showed significantly better results on the change of liquid fraction than the correlations previously reported in the literature. In the study by (Kim et al., 2019), a new effective thermal conductivity model was proposed and employed by the authors to investigate a tank designed for latent-heat TES (LHTES). The tank was filled with spherical capsules containing PCM arranged in a 9 x 9 x 20 distribution. Previous studies had primarily focused on evaluating the performance of a single capsule under the assumption that its performance could represent the entire tank. However, given the inherent complexity of phase-change analysis, even for a single capsule, analysing a whole tank was challenging due to the enormous amounts of calculation time and the memory capacity required. Throughout the entire melting process, the simulation results showed a close agreement with the experimental measurement.

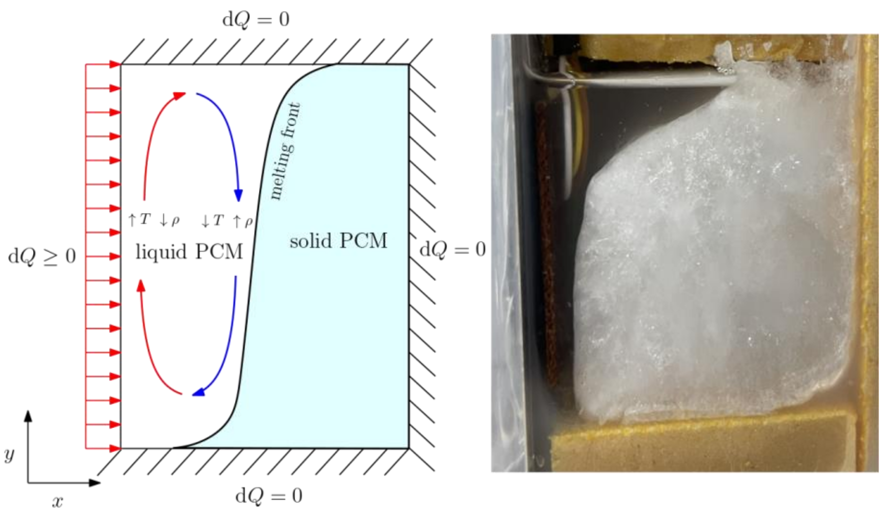

Figure 1: Convective flow pattern in a rectangular cavity: (a) schematics and (b) experiment

The purpose of the present study was to develop a computational heat transfer model that utilises an explicit finite difference method to simulate heat conduction, as well as a novel effective thermal conductivity function to model heat convection. As an initial step during the investigation of natural convection in liquid PCM, we employed and modelled the effective thermal conductivity-based approach as a linear function of the cavity height. The presented set of experiments and simulations also represents the first step towards the solution of inverse heat transfer problems in this area. The effective thermal conductivity approach is a less computationally demanding approach to the solution of heat transfer problems, involving phase change with natural convection, than other approaches, such as computational fluid dynamics, while still providing acceptable accuracy. The model was validated by experimental data (melting of a PCM enclosed in a rectangular cavity with a heated vertical wall). Rubitherm RT 35 HC, an organic paraffin-based PCM, was used in the experiments and temperature measurements were used to verify the accuracy of the proposed modelling approach.

2. Methods

2.1 Experimental set-up

The study involved the melting of a PCM sample contained within a rectangular cavity. The experimental setup enabled the application of a specific heat flux to one of the PCM sample's surfaces. Peltier cells were utilised to control the temperature on the heated surface and induce both melting and solidification of the material. A 3D-printed socket grid housed three Peltier cells in a uniform one-by-three distribution, positioned between the aluminium plate and a passive cooler. To ensure uniform temperature distribution, three Pt100 temperature sensors were embedded in the aluminium plate. Seven Pt100 sensors were placed within the PCM with 5 mm intervals between sensors to monitor temperature distribution along the PCM's thickness (with the exception of the last sensor, which was at a distance of 40 mm from the heated surface, as shown in Figure 2b). The paraffin-based Rubitherm RT 35 HC was used to fill the cavity, which had the dimensions
250 x 30 x 45 mm. A thermal insulation layer was employed to cover all outer surfaces of the setup, and two heat flux meters manufactured by AHLBORN, equipped with an integrated temperature sensor, were attached to the inner surface of the aluminium plate. A 2D numerical model was implemented, leveraging the symmetry of the setup along the length of the heated plate. The investigated scenario consisted of heating and cooling phases with 0.64 h and 1.63 h duration. Experimentally measured temperatures are shown in Figure 2a.

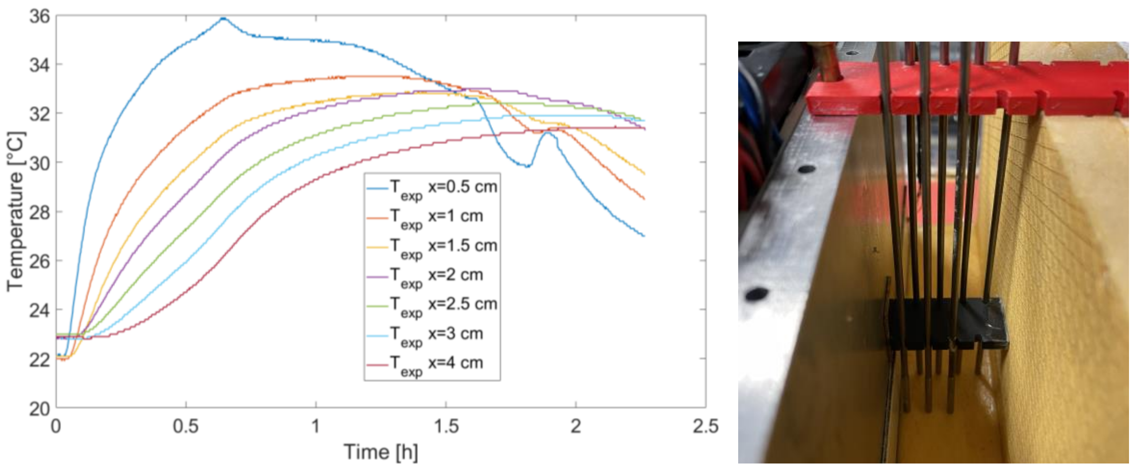

Figure 2: (a) Experimentally measured PCM temperatures (b) empty cavity with RTD sensors

Table 1: Parameters of the numerical model and material properties

Parameter	Symbol	Value	Unit
Cavity height	H	0.03	[m]
Cavity thickness	d	0.045	[m]
Latent heat	L_f	210	[kJ/kg]
Specific heat capacity	c	2,000	[J/(kg K)]
Phase change temperature	T_{PCH}	35	[°C]
Skewness in solid phase	σ_s	0.4	[K]
Skewness in liquid phase	σ_ℓ	0.6	[K]
Thermal conductivity in solid phase	k_s	0.2	[W m^{-1} K^{-1}]
Thermal conductivity in solid phase	k_{max}	4.2	[W m^{-1} K^{-1}]
Time discretization step	Δt	0.1	[s]
Density	ρ	800	[kg/m^3]
Number of nodes in *x*-direction	N_x	90	[-]
Number of nodes in *y*-direction	N_y	20	[-]

2.2 Numerical model

The numerical model of the cavity filled with the PCM was based on the solution of the 2D heat conduction problem. Similar approach was already used in the previous studies of the authors (Zálešák et al., 2021). The heat transfer equation in the PCM is considered in following form:

$$\mathrm{c}_{\mathrm{eff}}(T)\,\rho\,\frac{\partial T}{\partial t} = \nabla(k_{\mathrm{eff}}(T)\,\nabla \mathrm{T}) + Q, \tag{1}$$

where ρ describes the density of the PCM, T is the temperature, t is time, $k_{\mathrm{eff}}(T)$ is the effective thermal conductivity function, $\mathrm{c}_{\mathrm{eff}}(T)$ is the effective heat capacity function and Q represents any heat sources or sinks within the system (in the considered scenarios Q = 0). This equation describes the conservation of energy within the PCM and was solved numerically using the explicit finite difference method (based on energy balance) to obtain the temperature distribution within the cavity over time.
As for the phase change modelling, the effective heat capacity method was adopted. This method is based on using the specific heat capacity as a function of temperature. The $\mathrm{c}_{\mathrm{eff}}(T)$ function is usually defined in form of the Gaussian function with various degree of asymmetricity. One of the possible definitions is based on analogy to the two-piece normal distribution (TPND) using the definition adopted from (Wallis, 2014):

$$\mathrm{c}_{eff}(T) = \begin{cases} c_s + (\sigma_\ell - c_s)\xi(T) + \mathrm{A}\, e^{\frac{-(T-T_{\mathrm{PCH}})^2}{2\,\sigma_s^2}} & for\ T \le T_{PCH}, \\ c_s + (\sigma_\ell - c_s)\xi(T) + \mathrm{A}\, e^{\frac{-(T-T_{\mathrm{PCH}})^2}{2\,\sigma_\ell^2}} & for\ T \ge T_{PCH}, \end{cases} \tag{2}$$

where $A = L_{\mathrm{f}}\sqrt{\frac{2}{\pi}}(\sigma_\ell + \sigma_s)^{-1}$ is the scaling factor, the enthalpy of fusion is denoted as L_{f}, T_{PCH} is the phase change temperature, the liquid fraction of PCM signified by $\xi(T) \in [0{,}1]$, c_s and c_ℓ are the specific heat capacities in solid and liquid states, and skewness parameters in both solid and liquid states are denoted as σ_s and σ_l. This approach utilises two normal distribution probability distribution functions (PDFs) with parameters N($\mu = T_{\mathrm{PCH}}$, σ_s) and N($\mu = T_{\mathrm{PCH}}$, σ_l) by scaling both of them down to their common value of $\mathrm{c}_{\mathrm{eff}}(\mu = T_{\mathrm{PCH}}) = A$. This means that the solid and liquid PDFs are scaled by $\frac{2\sigma_s}{(\sigma_s+\sigma_\ell)}$ and $\frac{2\sigma_\ell}{(\sigma_s+\sigma_\ell)}$.
Similar approach was used for the definition of the effective thermal conductivity function, which was defined as both the function of PCM temperature and the function of the position within the cavity. As heat convection only occurs in the liquid phase, one of the restrictions on the effective thermal conductivity could be easily described as an if condition ($T \ge T_{PCH}$). Once this condition is fulfilled, the effective thermal conductivity function is defined as:

$$k_{\mathrm{eff}}(T,j) = k_{\mathrm{s}} + (k_{\max} - k_{\mathrm{s}})\frac{j}{\mathrm{N}_y},\ \ \text{if}\ (T \ge T_{PCH}), \tag{3}$$

where $k_{\max}$ is the maximum value of the effective thermal conductivity function, $j \in [1, N_y]$ is the index of the node and N_y is the total number of nodes, both in the *y*-axis direction. Equation 3 represents the relationship between the effective thermal conductivity and the height of the heated cavity, specifically for the molten phase of the PCM. Essentially, when the cavity is near the bottom (indicated by $j = 1$), there is a negligible change in the value of the effective thermal conductivity. However, as the height within the cavity increases, there is a linear growth, reaching the maximum value of $k_{\max}$ at the top (corresponding to $j = \mathrm{N}_y$). It's important to note that Equation 3 is applicable only when the PCM being studied is completely in its liquid state.

3. Results and discussion

Figure 3 displays the temperature evolution and phase change front in the vicinity of the heated surface, up to a depth of 1.5 cm, assuming constant thermal conductivity. It should be noted that the simulated temperatures (T_{sim}) depicted in Figure 3b are the average temperatures along the y-direction at a specific distance from the heated surface. The results indicate that the simulated temperature is overestimated in comparison to the experimental measurements. This discrepancy can be attributed to the influence of natural convection, which leads to an asymmetrical temperature distribution that is not accounted for in this instance.
On the other hand, if a linear increase in thermal conductivity is introduced (with the peak value of $k_{\max} = 4.2$ W m^{-1} K^{-1} at the top of the cavity as per Eq. 3), which accounts for natural convection, a noticeable enhancement in the precision of the numerical model can be observed in Figure 4. To assess the accuracy of a modelling approach, the root mean square error (RMSE) defined as

$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{N_{pt}} \sum_{p=1}^{N_{it}} \frac{\left(T_{\mathrm{sim,i}}^{p} - T_{\mathrm{exp,i}}^{p}\right)^{2}}{N_{pt}\, N_{it}}}, \tag{4}$$

where $N_{pt} = 7$ is the overall number of RTD sensors within the PCM volume, N_{it} is the total number of iterations, T_{sim}^{p} describes simulated temperatures and T_{exp}^{p} corresponds the experimentally measured temperatures. In the scenario where natural convection was not considered, the RMSE was found to be 4.0 K. However, when using the proposed effective thermal conductivity approach, the RMSE significantly reduced to 1.9 K, representing a 47.5 % decrease in error. The uncertainty of temperature measurements (Pt100 probes connected to a datalogger) was 0.1 K. The RMSE lies outside the uncertainty range of temperature measurements. The uncertainty of heat flux measurements was ±5 %. There was a higher discrepancy between the measured and simulated PCM temperatures when the heat flux was used as the boundary condition. Therefore, only the results for the heated surface temperature as a boundary condition are presented in the paper.
The present version of the adopted approach is only applicable for the studied case (melting process in an enclosed cavity of given dimensions). The application of inverse identification procedures to acquire the effective heat conductivity distributions (with regard to the dimensions, heat fluxes, temperature gradients, etc.) is expected to generalize the approach for other cases.

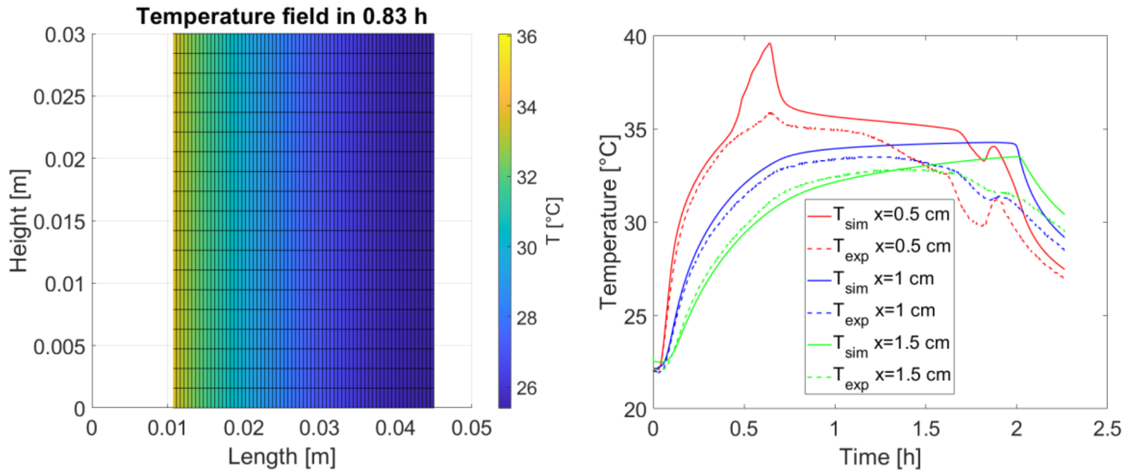

Figure 3: (a) Phase change front after 0.83 h and (b) temperature evolution near the heated surface for constant thermal conductivity $k_{max} = k_s$

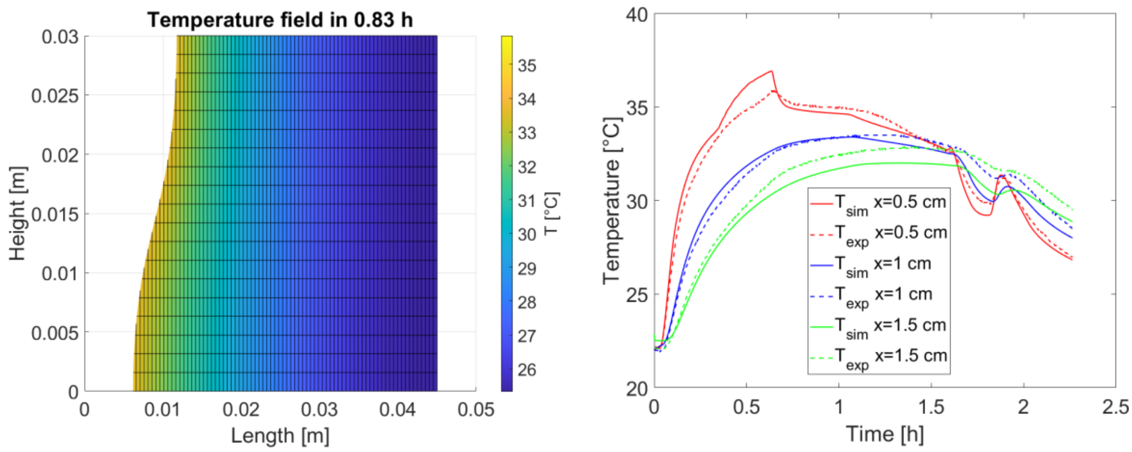

Figure 4: (a) Phase change front after 0.83 h and (b) temperature evolution near the heated surface for effective heat conductivity with linear increase along the cavity height $k_{max} = 4.2 \geq k_s$

4. Conclusions

An approach based on effective thermal conductivity is introduced for modelling of convective heat transfer within a liquid PCM. The findings of the research can be outlined as follows:

- A comprehensive experimental setup was designed to investigate thermal behaviour of PCMs, and pilot experiments were performed.
- A two-dimensional numerical model of heat transfer with phase change was established using the explicit finite difference method, coupled with the effective heat capacity approach.
- As a part of the investigation of thermal behaviour during natural convection, a novel approach based on effective thermal conductivity was introduced, which employs a linear increase in thermal conductivity along the height of the cavity (up to twenty times that of the thermal conductivity in the solid phase).
- The outcomes of the simulation indicate that incorporating the effective thermal conductivity approach significantly improved the precision of the numerical model. Specifically, a 47.5 % decrease in the root mean square error (RMSE) was observed between the experimental and simulated temperatures, as the RMSE decreased from 4.0 K to 1.9 K.

Nomenclature

A – scaling factor, J/(kg K)
c – specific heat capacity, J/(kg K)
c_{eff} – effective heat capacity, J/(kg K)
d – cavity thickness, m
k – thermal conductivity, W/(m K)
k_{eff} – effective thermal conductivity, W/(m K)
$k_{\max}$ – maximum value of k_{eff}, W/(m K)
L_f – enthalpy of fusion, J/kg
N_{it}– total number of iterations, -
N_{pt} – total number of RTD sensors, -
N_x, N_y – number of nodes in x and y direction, -
T – temperature of PCM, K
T_{pch} – peak temperature of phase change, K
Δt – time discretization step, s
x, y – cartesian coordinates
ρ - density of PCM, kg/m^3
σ_s, σ_ℓ – skewness coefficients of the c_{eff}, K
ξ – liquid fraction, -

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