Coupled thermo-fluidic model for thermal energy storage based on liquid solid phase change

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Abstract
The production and storage of thermal energy are important processes that contribute to the satisfaction of daily needs. They are effective ways of managing the thermal energy available from various solar applications. The most efficient storage technique is the use of phase change materials (PCMs) because these components can keep large amounts of thermal energy in stock. The problem is that this approach continues to be confronted with difficulties despite significant progress in research, design and modelling. Nevertheless, these difficulties can be resolved through numerical simulations that enable the identification of powerful tools for optimising thermal system design and predicting thermal behaviour. Correspondingly, in this work, thermo-mechanical modelling was conducted to describe the different methods of heat transfer that can optimise thermal energy storage via PCMs. This study also established a numeric resolution and the spatio-temporal discretisation of the basic equations accompanying the numerical model. The proposed numerical solution improves the prediction of thermal behaviour and can be used as a guide in designing new systems capable of producing and storing solar energy.

1. Introduction

In recent years, important improvements to thermal energy storage have occurred because of the development of storage techniques, especially those involving the use of latent heat. Latent heat storage is a solution that exploits the inactive heat produced during phase changes; that is, it capitalises on the ability of materials to transition from one state to another under the effect of temperature. One of the most important physical phenomena arising from latent heat storage is solid–liquid phase change, in which the energy from phase change is absorbed during the melting of a phase change material (PCM) and restored during solidification. Enhancing the interpretation of solid–liquid phase change necessitates determining temperature distribution in the solid and liquid phases, flow characteristics in the liquid phase, heat transfer characteristics and interface location. Solid–liquid phase change, however, is a complex process that combines natural convection with the liquid phase. For this reason, such phenomenon is a powerful non-linear process that is difficult to analyse, except in simple and ideal test cases.

The above-mentioned problems may be solved via PCM technology’s, which can be integrated into building envelopes, building components or structures (i.e. roofs, walls and floors) and can be installed in either passive or active systems. PCMs have recently been incorporated into various applications, attracting considerable interest from practitioners in the building, storage and cooling industries. These materials have also been used in domestic storage, especially water tanks [1]. Thereby improving thermal systems and reducing storage costs. Many researchers [2, 3] developed technologies for storing thermal energy in a tank without the use of a PCM that can stabilise a system, but they could not establish an effective backup strategy for thermal energy storage. To address this issue, Zhao et al [4] integrated a PCM in a thermal energy storage element to improve the production of a thermo-electric system. The integration approach was based on a mathematical study and
validated experimentally. Takeda et al\cite{5} studied PCM performance in the ventilation systems of buildings to identify materials that can reduce ventilation costs in different Japanese climates.

The current work formulated a numerical model that illustrates PCM behavioural responses to different methods of heat transfer that can optimise the storage of thermal energy in PCM systems. Simulations were conducted to identify a numeric resolution that delineates solid–liquid phase change and is based on the resolution of Navier–Stokes equations. The proposed resolution considers boundary conditions and the spatial-temporal discretisation of the governing equations of the numerical model. The proposed numerical solution improves the prediction of thermal behaviour and serves as a reference for optimising energy production and storage in thermal systems.

2. Modeling

The physical phenomena occurring in the area between a fluid and a PCM were modelled. The governing equations were used to identify the relationship between the heat equation and the Navier–Stokes equations that were adopted to a rectangular PCM plate. Assumptions and simplifications about thermo-physical properties of PCMs and boundary conditions were established, paying attention to every modes of heat transfer. The resolution implemented through coupled modelling was then used to determine the association amongst the speed, pressure, temperature and density of a moving fluid.

The equations in this study have been shortened, for more details the reader can return to the supporting information (SI) is available online at stacks.iop.org/MRX/7/025516/mmedia accompanying the paper in order to understand the changes and the transformations between the steps in the equations.

2.1. Physical model

The early stage of the fusion process is governed by conduction and radiation. On the one hand, when liquid fraction increases, convection develops and dominates heat transfer; on the other hand, in the unmelted solid phase, conduction remains the principal form of heat transfer. As long as the natural convection in the liquid phase is maintained, it causes faster melting in the upper part of a PCM than in lower parts, which eventually changes the form of the solid–liquid interface (figure 1).

Variations in material volume during phase change were assumed to be negligible, the PCM of interest was assumed to be homogeneous, isotropic and thermo-physical properties were assumed constant. The system is depicted in figure 2.

The system in figure 2 describes the boundary conditions for thermal energy storage in a PCM layer with thickness $E$ and height $L$. To investigate the interaction between heat transfer fluid and the PCM in a rectangular cavity under a stationary regime, the system was designed in a way that allows the top surface to receive hot temperature and the bottom face to receive cold temperature. The rest of sides has been assumed adiabatic (figure 2).
2.2. Heat transfer in PCMs

Over the past 20 years, liquid–solid phase change has been examined using numerical and experimental methods, and this phenomenon was assumed a very complex and nonlinear problem, which associates three fundamental phenomena: the natural convection in the liquid-phase, the heat conduction in the solid phase and solar radiation.

Improving the thermal conductivity of PCMs is apparently the most direct way to improve heat transfer. However, many studies have shown that the neglect of other modes of heat transfer compared to conduction negatively affects the melting/solidification process, the best example being the importance of convective heat transfer in the melting PCM process.

It is therefore clear that conduction alone is not adequate, as other modes of heat transfer [6] (radiation and convection) must be taken into account in the phase change processes of storage systems. Strategies to improve other modes of heat transfer, namely convection and radiation, open up new ways to optimize charge/discharge duration.

In this part, the various modes of heat transfer that affect the PCM layer has been developed:

- Thermal conduction, \( \varphi_{\text{cond}} \)
- Thermal convection, \( \varphi_{\text{conv}} \)
- The radiation, \( \varphi_{\text{ray}} \)

The flux of surface balance is expressed as the sum of the fluxes applied to the surfaces, the different flows are:

- the conductive flux between the surface and the node of PCM closest to the surface, the convective flux between the surface and the outside air and the radiation flow:

\[
\varphi_{\text{tot}} = \varphi_{\text{cond}} + \varphi_{\text{conv}} + \varphi_{\text{ray}}
\]  

2.2.1. Thermal conduction

The conduction can transfer the heat in the material that realized without macroscopic movement of the material, under influence of a temperature difference. The heat flux transmitted by conduction can be written according to the Fourier law by the following equation:

\[
\varphi = -K \frac{S \text{grad} T}{\text{°C}}
\]  

With: \( \Phi \): Conducted heat flux (W), \( K \): Thermal conductivity (W m\(^{-1} \) °C\(^{-1} \)), \( S \): section Area of heat flow (m\(^2 \)) and \( T \): temperature of the fluid in (°C).

The minus sign denotes that heat transfer is in the direction of decreasing temperatures.

The literature on the melting and solidification processes of PCM shows that heat conduction is the main mechanism of heat transfer during the solidification process, while natural convection performs a dynamic role during the melting process.
2.2.2. Thermal convection

Convection is the transfer of heat in the material with a macroscopic displacement of the material, due to the differences of densities caused by too great differences of temperatures. The convective energy transfer can be happened in the fluid-solid interface that can be expressed in a practical way by Newton’s law of cooling.

\[ \varphi = h \left( T_p - T_\infty \right) \]  

(3)

With:

- \( \varphi \): Heat flow transmitted by convection (W),
- \( h \): Coefficient of heat transfer by convection (W.m\(^{-2}\).°C\(^{-1}\)),
- \( T_p \): Solid Surface Temperature (°C),
- \( T_\infty \): Fluid temperature far from the surface of the solid (°C),
- \( S \): Area of contact solid / fluid (m\(^2\)).

There are two kinds of convection: natural and forced convection. The first one, natural convection or free convection for which the movement of the fluid results directly from the existence of temperature and density gradients in the fluid. The second one, the convection has been forced the circulation of a fluid by a device (pump, compressor, and turbine) the heat transfer is faster than that of natural convection.

Recently, the solid–liquid phase change of PCM in various geometrical measures with natural convection in the liquid phase has been investigated theoretically and experimentally. Thermal energy is stored in the PCM as latent heat and is reused when needed. Therefore, the understanding of natural convection inside the PCM liquid acting significant rules in the design of the thermal storage system.

Tan et al. [4] studied experimentally the phenomena of buoyancy and natural convection during the fusion of a PCM in a spherical capsule. These results were confirmed with a numerical solution obtained using CFD Fluent software. Tan et al. showed that conductive heat transfer predominated initially, while buoyancy-induced convection became more important as the volume of the liquid fraction increased. However, the melted PCM is mounted upward in the upper regions of the sphere due to natural convection. As a result, the upper regions of the sphere melted first, followed by other regions. Another interesting conclusion of the computational results is that the temperature distribution has fluctuated chaotically at some points of the sphere, due to the presence of the unstable fluid layer at these points.

2.2.3. Radiation

It is the transport of heat in the form of electromagnetic waves. The heat passes from a body at high temperature to a body at low temperature in the form of electromagnetic radiation (photon), the two bodies must be in a transparent medium (such as air or vacuum). In conduction problems, it takes into account the radiation between a solid and the surrounding environment and in this case, we have the relationship:

\[ \Phi = \sigma \varepsilon_p S (T_p^4 - T_\infty^4) \]  

(4)

With: \( \Phi \): Radiant heat flux (W), \( \sigma \): Stefan’s constant (5.67 x 10\(^{-8}\) W.m\(^{-2}\).K\(^{-4}\)), \( \varepsilon_p \): Emission factor of the surface, \( T_p \): Surface temperature (K), \( T_\infty \): Temperature of the environment surrounding the surface (K) and \( S \): Area of the surface (m\(^2\)).

However, the improvement of radiation heat transfer deserves additional attention. As such, little attention has been given to thermal radiation as a mode of heat transfer in the melting/solidification of these materials. The potential for improving radiative transfer in these materials as an enhancement of heat transfer will therefore be discussed as a separate category [7].

2.3. Modeling

The physical properties of air (temperature, pressure) excepting density, are assumed to be independent of temperature throughout this study. Concerning the Archimedes principle, it has been chosen to describe the temperature dependence of the density using the Boussinesq approximation. This choice was made because the Boussinesq approximation correctly reflects the main heat transfer characteristics regarding small differences in temperature.

The equation system that governs the flow of a two-dimensional, incompressible fluid in laminar flow includes the equations of Navier–Stokes (mass conservation equation, momentum equation, and energy conservation equation) coupled with heat transfer equations (conduction, convection, radiation). Therefore, the governing equations can be written as follows:

2.3.1. Mass conservation equation

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \]  

(5)

(u, v) velocity vector in x and y directions respectively.
2.3.2. Momentum conservation equation

Projection on x:

\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = - \frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \rho g \beta (T - T_\infty) + \frac{(1 - F)^2}{(F^3 - \xi)} A_m u
\]

With: \( P \) the pressure, \( \rho \) the density, \( \beta \) coefficient of thermal expansion, \( \mu \) dynamic viscosity, \( g \) acceleration of gravity, \( F \) liquid fraction, \( A_m \) constant of the pasty zone and \( \xi \) real number of low value \((10^{-4})\) to avoid division by zero and \( T \) temperature.

Projection on y:

\[
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = - \frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \rho g \beta (T - T_\infty) + \frac{(1 - F)^2}{(F^3 - \xi)} A_m v
\]

2.3.3. Energy conservation equation

\[
\frac{\partial (\rho H)}{\partial t} + U_x \frac{\partial (\rho H)}{\partial x} + U_y \frac{\partial (\rho H)}{\partial y} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + r
\]

The systems undergoing a phase change have a total enthalpy equal to the sum of the sensible energy \( h_s \) and the latent energy \( h_L \) as presented in the equation (9) below:

\[ H = h_s + h_L = \int c_p dT + F L_F \]

The sensible heat \( h_s \) corresponds to the stored energy as a rise in the temperature of the solid or liquid material and can be expressed by equation (10) below:

\[ h_s = \int c_p dT \]

With \( c_p \): The specific heat.

The latent heat \( h_L \) represents the energy accumulated by the material during its phase change and can be expressed according to equation (11) below:

\[ h_L = F L_F \]

With \( L_F \): Latent heat absorbed locally

F: The liquid fraction defined by:

\[
F = \begin{cases} 
0 & (T < T_{sol}) \\
\frac{T - T_{sol}}{T_{liq} - T_{sol}} & (T_{sol} \leq T \leq T_{liq}) \\
1 & (T > T_{liq})
\end{cases}
\]

\[
\frac{\partial (\rho \int c_p dT + F L_F)}{\partial t} + u \frac{\partial (\rho \int c_p dT + F L_F)}{\partial x} + v \frac{\partial (\rho \int c_p dT + F L_F)}{\partial y} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + r
\]

It can be determined that the final equation is:

\[
\rho c_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \rho L_F \left( \frac{\partial F}{\partial t} + u \frac{\partial F}{\partial x} + v \frac{\partial F}{\partial y} \right) + r
\]

for more supporting information.

2.4. Coupling thermo-fluidic

The phenomenon of solid-liquid phase change is a complex process that couples thermal and hydraulic phenomena, through the equation of heat and the Navier–Stokes equations. For these causes, the phase change of solid–liquid is a powerful non-linear process, and hard to analyse, excluding for ideal and simple test cases.

The phase change in the PCM occurs by the different heat transfers, especially the heat due to solar radiation including the other heat sources (conduction-convection) that appear in the system of interaction between fluid-PCM.
be optimise the maximum melting time-saving ratio of PCM. Additionally, the storage of thermal energy in the PCM can be quantified in terms of the radiation transfer mode. As a result, a comparison has been made which showed the possibility of a modelling that explains the simplification and assumptions of the PCM configuration are given in table 1.

| Property             | Methyl palmitate | Paraffin wax | Aluminium | Air |
|----------------------|------------------|--------------|-----------|-----|
| Density (kg/m³)      | 852              | 834.36       | 2719      | 1.22|
| Specific heat (J/kgK)| 1.75             | 2890         | 871       | 1006.43|
| Thermal conductivity (W/m.K) | 0.179          | 0.22         | 202.4     | 0.0242|
| Melting heat (J/g)   | 229.5            | 70.10⁻³      | —         | —   |
| Solidus temperature (K) | 292           | 292          | —         | —   |
| Liquidus temperature(K) | 300            | 300          | —         | —   |

It is assumed that the change in PCM volume during the modification phase was negligible $\Delta V = CST$. In addition, the PCM is isotropic, homogeneous and the thermo-physical properties are assumed constant. By considering, the equation (14) that can be written as the following equation:

$$\rho c_p \left( \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} \right) = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \rho \lambda \left( \frac{\partial F}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} \right) + \varphi_{ray}$$  \hspace{1cm} (15)

It is defined that $r$ (internal source) with relation:

$$r = \varphi_{ray}$$  \hspace{1cm} (16)

With $\varphi_{ray}$, the flux of the Sun radiation,

$$\rho c_p \left( \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} \right) = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \rho \lambda \left( \frac{\partial F}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} \right) + \varphi_{ray}$$  \hspace{1cm} (17)

$$\varphi_{ray} = \sigma e_p S(T_p^4 - T_{\infty}^4)$$  \hspace{1cm} (18)

By replacing the radiation flux by its expression in equation (17) above:

We obtain:

$$\rho c_p \left( \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} \right) = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \rho \lambda \left( \frac{\partial F}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} \right) + \sigma e_p S(T_p^4 - T_{\infty}^4)$$  \hspace{1cm} (19)

The coupled thermal and fluidic model describes the solid-liquid phase transformation by basing on the radiation transfer mode.

It can be concluded that the modelling able to present the simplifications and assumptions of the PCM behaviour and the different modes of heat transfer. Additionally, the storage of thermal energy in the PCM can be optimise the maximum melting time-saving ratio of PCM.

### 3. Results and discussion

The numerical model can predict the PCM behaviour paying attention to every mode of heat transfer. The numerical model solution can improve the prediction of the thermal behaviour and can be used to optimize and to reduce the production and storage time in thermal systems.

The accuracy of equations of the numerical model needs to be validated. For this purpose, the model has been tested in the Platform Matlab, which can validate the proposed modelling. The properties of the studied configurations are given in table 1. As a result, a comparison has been made which showed the possibility of a modelling that explains the behaviour of materials, which largely corresponds to the references [10, 11], with a significant improvement in the current results, by dint of taking into account all heat transfer as an extra thermal energy.

In the beginning, the results describe the enthalpy versus temperature. The simulation curve is divided into three parts: initially, the PCMs absorb significant amounts of heat energy that is stored as sensible heat. Hence, the temperature increases until they reach the temperature of the phase change (melting temperature). However, the PCMs absorb heat until all materials are converted to the liquid phase. It can be observed that the proposed model describes accurately the phase change. Therefore, the results are improved when including different heat transfers which lead to a rapid phase change of the PCM. Thus, the melting time is optimised and more amount of energy is collected as shown in figure 3.

The specific heat of solid state is the slope of the enthalpy-temperature curve before the phase transition zone (sensitive heat of solidification). Similarly, the specific heat capacity in the liquid state is the slope after the phase transition zone (sensitive heat of melting). Despite the increase in the specific heat capacity and overall energy of...
the storage system, which theoretically should increase the melting/solidification time, the reduction of the melting/solidification time is attributed to a higher overall heat transfer rate due to the aforementioned increase.

Every source of energy is considered as an extra energy that improves the collection of thermal energy, which can speed up the PCM heating, consequently, reducing melting time as shown in figure 4:

The slope of the temperature during the solid to liquid (melting) cycle declines for the first 30 min, and then becomes almost straight at around 30 min to 120 min. During this period, the solid to liquid (melting) phase transition takes place at 24.5°C. The PCM stores energy with the increase of temperature. Otherwise, solidification begins subsequently the temperature decreases well below the phase change temperature. It can be concluded that the simulation predicted the melting/solidification temperature of the PCM system and it is in

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**Figure 3.** The evolution of enthalpy $H$ as a function of temperature.

**Figure 4.** Curve of temperature versus time with comparing the model and literature [10].
good agreement with the literature\cite{10, 12, 13}. Additionally, the model is taking all heat transfers that present a significantly improvement in melting time and the stored energy.

The agreement between experimental and calculated graph has permitted a validation of the proposed model and deduces some unreachable values such as the evolution of the liquid fraction versus time.

Figure 5 shows numerical simulations of the fraction liquid as function of time for melting and solidification processes. The proposed numerical model describes correctly the two opposite processes and the study of solid-liquid phase change focuses on the boundary conditions and physical properties of the final solid product\cite{6, 14}.

The variation of temperature as a function of time stores a large amount of energy in the system as can be seen in the figure 6:

Figure 6 shows that the energy initially stored increases as the temperature increases over time, then the energy is stable when the temperature stops increasing. Later on, the stored energy decreases when the temperature of the PCM decreases after use or the temperature of the environment decreases, which causes a decrease in the temperature in the system.
The effect of heat flow on charging process has been studied in many previous literatures \[10, 12\]. Some authors have mentioned that heat flow has a significant influence on the charging process. The heat flow and the average temperature of the PCM under different heat flow rates are illustrated in figure 7.

Figure 7 shows the heat flow through the PCM as a function of the temperature. The simulation describes the energy absorbed and released during the phase change (solidification/fusion). Hence, the proposed model shows significant improvement about phase change temperature by paying attention to every source of energy, which has been discarded in most studies.

In order to improve the production and the storage of thermal energy, a 2D numerical simulation using ANSYS FLUENT software based on finite volume approach is proposed.
In addition, the Paraffin wax [14] is used in the melting process that had an important latent heat and can be found everywhere. The geometrical model is uniformly meshed using symmetric square cells as depicted in figure 8. A very fine mesh was applied to the 2D square PCM, which predicting correctly its features. The selected elements are 40 000 and the nodes are 40401.

In order to improve the computational efficiency of 2D model with double precision is used. In addition, the control parameters are used by default. Furthermore, the SIMPLEC method is adopted in pressure, velocity coupling mode, the mode of retention is PRESTO method, and the rest are all defaults [14, 17].

At first, the heat transmits through the PCM by different heat transfers due to the temperature dissimilarity between the system temperature and the PCM. Right after the 30th minute (figure 9), the absorbed heat is then used to phase change from solid state to a liquid state. After beginning of fusion phase, the natural convection and conduction are contemporary in the system. Therefore, there is an increase of the melting process, and the natural convection. Then, half of the PCM is melted after the 80th minute.

The results make it possible to describe the real behaviour of phase change over time, which is in good agreement with the results of the literature [14]. Although several works discussed the engineering and the importance of geometry and the effects of geometry part in the melting process of PCM, the present study is destined for rectangular PCM and engineering issues are intended for next works to improve the ability of this model.

Figure 9. Temporal evolution of the PCM melting in the collector (from top to bottom) (10, 20, 30, 40, 50, 60, 70, 80, 100, and 120 min) [6, 14].
4. Conclusion

The PCM is a material that can store a large amount of heat to use it when needed. In this work, thermo-mechanical modelling was conducted to describe the different methods of heat transfer that can optimise thermal energy storage via PCMs. On the one hand, the simulations present the numeric resolution that describes the solid-liquid phase change which is based on the resolution of the Navier–Stokes equations, taking into consideration the boundary conditions and spatial-temporal discretisation of the governing equations of the numerical model. Therefore, a detailed comparison has been made between the results and literature. This comparison has shown they are in good agreement with each other. However, a significant improvement at the level of collected energy and the storage time via the phase change has been achieved when we added the extra energy that comes from all heat transfers.

On the other hand, the simulation using ANSYS software has been made by well-structured mesh and adapted to the geometry. The numerical results are describing the phase change of a real behaviour of PCMs. The numerical solution can improve the prediction of the thermal behaviour and can benefit from the extra energy coming from the different methods of heat transfers that optimize production and storage in thermal systems compared to the previous systems.

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