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ORIGINAL RESEARCH PAPER

CFD modeling for phase change materials integrated to building envelope

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ABSTRACT

Integrating thermal energy storage with thermal conversion systems is necessary to maximize their use. Phase change materials are the best media for storing and releasing thermal energy from various basic material types. Because the phase change materials have a high latent heat of fusion, it is often viable to use these characteristics and include the phase change materials in building envelopes to store thermal energy. The paper provides a thorough categorization of the phase change materials and thermal energy storage systems, in addition to an evaluation of their modeling using computational fluid dynamics. The purpose was to highlight computational fluid dynamics as a useful technique for advancing the engineering of thermal energy storage devices.

KEYWORDS

phase change materials, thermal energy storage, latent heat storage, computational fluid dynamics, energy consumption

1. INTRODUCTION

The most challenging issue in most countries is the global energy consumption in buildings. The International Energy Agency (IEA) reports that the overall energy consumption for buildings worldwide has lately climbed to 40% for commercial buildings and 61% for residential buildings. Heating, Ventilation, and Air Conditioning (HVAC) utilize the most energy. The energy used by buildings is predicted to rise by up to 37% in 2050 if this trend continues [1]. Maintaining a comfortable atmosphere is one of the top priorities for commercial and residential buildings, which places particular demands on heating and cooling energy. Between 20% and 40% of the total energy demand is used by buildings [2, 3]. Therefore, improving system efficiency would significantly reduce energy use. Good thermal management is necessary to guarantee system effectiveness. Thermal energy can be stored instead of lost through Thermal Energy Storage (TES) systems, a recent advancement in thermal management technology. There are numerous ways to implement this technology, including storing energy via a thermochemical process and using sensible and latent heat [4]. Phase Change Materials (PCMs) are used in the Latent Heat Storage (LHS) system [5]. Studies on the thermo-physical characteristics of various PCMs and strategies for incorporating them into building envelopes have been published by several researchers. Experimental and numerical studies of these materials' thermal energy storage capabilities have been conducted [5–11]. Utilizing Computational Fluid Dynamics (CFD) is anticipated to be a practical method for providing optimization tools for the optimal efficiency of these systems while also saving money and time.

This study focuses on using CFD to model and simulate thermal energy storage in phase change materials embedded in building envelopes.

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2. CLASSIFICATION OF PCMS

Phase change materials store thermal energy and release it during the phase change from a liquid state to a solid state at a constant temperature as it can be seen in Fig. 1. This feature of phase-changing materials can be exploited to regulate thermal energy in buildings and reduce its consumption [12, 13].

In general, phase change substances are divided into three classes based on their chemical composition: organic, inorganic, and eutectic. Each category is characterized by thermal and physical properties that enable researchers to choose the most appropriate option, according to the intended application [14].

Most paraffin is made up of hydrocarbons. The biggest phase transition material category is fatty acids, not paraffin. Metallic and salt hydrate PCMs are the two categories of inorganic PCMs. While undergoing a phase shift, hydrate salts are both hydrated and dehydrated, although not all hydrate salts melt simultaneously. Metallic is eutectic metal with low melting points. Although these metallic is highly light and has a high thermal conductivity similar to metal, it has low latent heat of fusion. Eutectics are an additional option for PCMs. Eutectics are mixtures of two or more substances, including organic and organic, inorganic and inorganic, or organic and inorganic. The solution to the melting of hydrate salts has been found via eutectics. Incongruent melting may be avoided while also lowering the melting point and improving the thermal conductivity by combining two kinds of hydrated salts, such as inorganic and inorganic salts, to create a eutectic.

3. PCM NUMERICAL SOLUTION

Numerous studies have been performed on heat transfer in PCMs incorporated within building envelopes. In this section, numerical and analytical solutions and the use of CFD for these problems are explored.

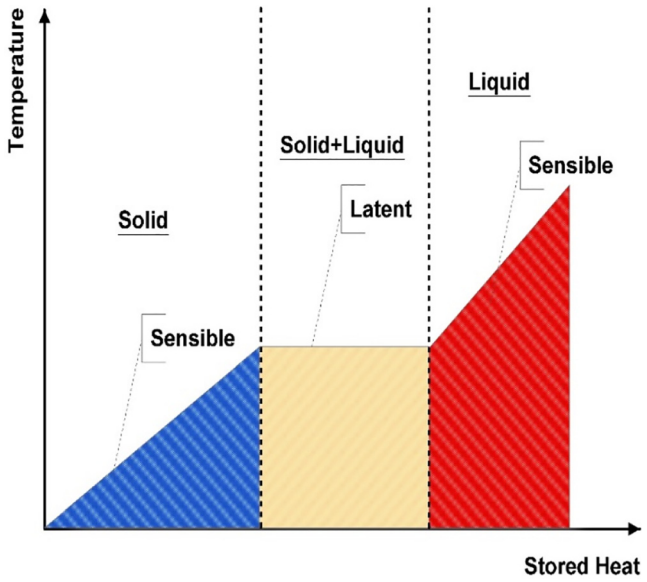

Fig. 1. Heat stored during phase transition (*Source*: Author's)

CFD may be useful for improving the engineering development of thermal energy storage systems. Additionally, it is anticipated that using CFD would provide optimization tools for these systems' maximum efficiency and a cost- and time-saving method.

A partial differential equation (PDE) that can be solved analytically or numerically governs how a phase transient, also known as a phase change, is mathematically formulated. The nonlinear phase front interfaces, complicated geometries, and nonstandard boundary conditions make it challenging to solve PCMs analytically. There are a few studies that have been conducted on 1D examples with regular geometries and a common boundary condition. The nonlinearity of numerical solutions at moving interfaces, where the displacement rate is governed by latent heat lost or absorbed at the boundary, makes it challenging to solve.

However, two primary approaches may be used to analyze the heat transport processes in solid-liquid PCMs:

- *Enthalpy-based:* The solid-liquid interface location need not be monitored in this manner. Because of the following benefits an enthalpy formulation is frequently used: No explicit requirements must be met at the solid-liquid interface; the governing equation is comparable to that of a single phase; the enthalpy formulation involves the solution in a mushy zone between the two standard phases that contains both solid and liquid components; It is simpler to handle the phase change issue, as it is shown in Eq. (1),

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \boldsymbol{v} H) = \nabla \cdot (k \nabla T) + S, \tag{1}$$

where H [J kg^{-1}] is the enthalpy of material; ρ [kg m^{-3}] is the density of material; T [°C] is the temperature; k [W m^{-1} K] is the thermal conductivity; $\boldsymbol{v}$ [m s^{-1}] is the velocity of fluid; S is the source term.

- *Temperature-based:* The only dependent variable in this approach is temperature. Since the solid-liquid interface location can be precisely recorded, the energy conservation equations for the solid and liquid may be stated independently. This allows for an accurate solution to the issues, as it is shown in Eq. (2),

$$\frac{\partial T_s}{\partial n} \cdot k_s = \frac{\partial T_L}{\partial n} \cdot k_L + \rho \cdot H \cdot k \cdot v_n, \tag{2}$$

where T_S [°C] is the solidus temperatures of PCM; T_L [°C] is the liquids temperature of PCM; k_s [W m^{-1} K] is the thermal conductivity of solid phase; k_L [W m^{-1} K] is the thermal conductivity of liquid phase; $\boldsymbol{n}$ is the unit normal vector to the interface; v_n is the normal component of the velocity of the interface; H [J kg^{-1}] is the enthalpy of material.

4. CFD ANALYSIS

Researchers utilize self-developed programs using language (C++, Fortran, MATLAB, and several commercial software

like COMSOL Multiphysics and Fluent by ANSYS) to simulate melting and solidification processes in engineering difficulties as well as the heat transmission phenomena in PCMs [15–17]. This research uses ANSYS Fluent software to simulate melting and solidification processes in engineering applications and the heat transmission phenomena in PCMs.

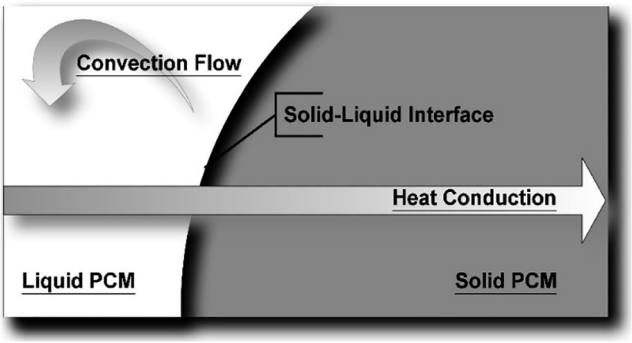

Fig. 2. Enthalpy porosity approach (*Source*: Author's)

Engineering challenges have been successfully simulated using the Fluent tool of the workbench ANSYS 2023 R1 [18]; it features a specialized model that can simulate a variety of various melting and solidification difficulties. The program may resolve phase changes across a wide temperature range or at a single temperature.

First, the physical engineering problem is mesh, particularly geometric modeling utilizing mesh creation tools, such as the workbench ANSYS 2023 R1. The boundary layers and zone types are established when the physical configuration is designed and meshed, and the mesh is sent to the Fluent program. To guarantee that the numerical results are independent of the parameters, several grid sizes, and time steps should be used for the numerical model. Small grid sizes and time increments are preferred for a quick computer simulation time.

ANSYS Fluent uses the enthalpy porosity approach to characterize the solidification and melting processes, as demonstrated in Fig. 2. This method does not specifically follow the melting interface. The liquid fraction, or the proportion of the cell volume that is liquid, is a value that is assigned to each cell in the PCM domain. The enthalpy

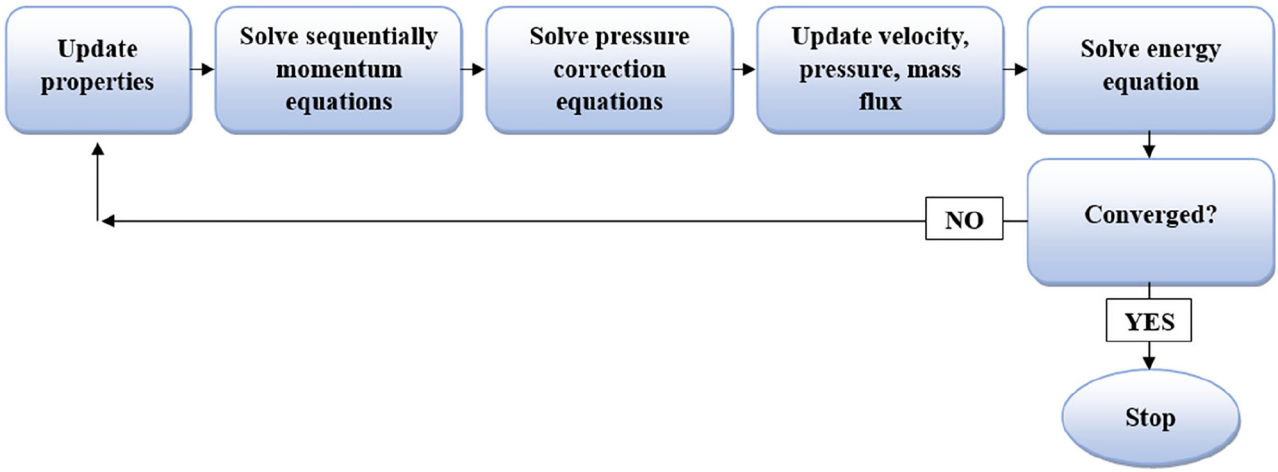

Fig. 3. Pressure-based flow chart (*Source*: Authors')

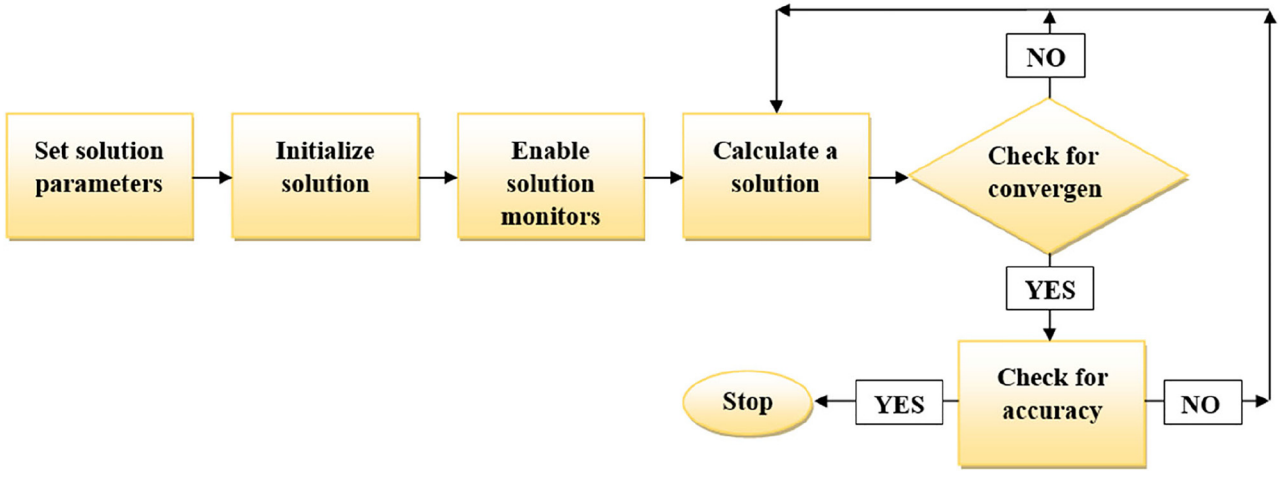

Fig. 4. Fluent solution flow chart (*Source*: Authors')

balance is used to calculate the liquid fraction after each repeat. This method's liquid fraction value ranges from 0 to 1, and the phase transition boundary is represented as a mushy zone. The mushy zone's porosity decreases from 1 to 0, similar to a pseudo-porous zone [19]. The porosity and velocity are zero when the material solidifies.

The energy equation is written as it is shown in Eq. (3) [19],

The sum of the sensible heat and the latent heat is employed to calculate the material's enthalpy,

$$H = h + \Delta H, \tag{3}$$

where h [J kg^{-1}] is the sensible heat; ΔH [J kg^{-1}] is the latent heat content, where

$$h = h_{ref} + \int_{T_{ref}}^{T} C_p \cdot dT, \tag{4}$$

where h_{ref} [J kg^{-1}] is the reference enthalpy; T_{ref} [°C] is the reference temperature; C_p [J kg^{-1} K] is the specific heat at a constant pressure of PCM.

The liquid-fraction (f) can be defined as:

$$f = \begin{cases} 0, & \text{if } T<T_S(\text{Solidification}), \\ \dfrac{T - T_S}{T_L - T_S}, & \text{if } T_S<T<T_L(M\text{ushy zone}), \\ 1, & \text{if } T>T_L(\text{Melting}), \end{cases} \tag{5}$$

where T_S [°C] is the solidus temperatures of PCM; T_L [°C] is the liquids temperatures of PCM.

The latent heat content can be written in terms of the latent heat of material as

$$\Delta H = f \cdot L. \tag{6}$$

The latent heat content can vary between zero (for a solid) and L (for a liquid) state.

The Fluent software has two main solvers: the pressure-based solver and the coupled density-based solver. The melting and solidification issues can only be simulated using the first technique. Two pressure-based solver algorithms, a segregated algorithm, and a coupled algorithm, are shown in Fig. 3. Both are included in Fluent.

For the convection terms in Fluent, many discretization strategies are available. Most often utilized with solidification and melting issues are the first order upwind, power law, and second-order upwind schemes. The solution technique overview is depicted in Fig. 4. More details about the solution, initialization, and discretization methods can be found [18].

Materials' physical characteristics, including density, thermal conductivity, heat capacity, and viscosity, may vary with temperature or rely on their chemical composition. A polynomial, piecewise linear or piecewise-polynomial function is the foundation for temperature dependence. Either the user defines or computes each component's attributes using kinetic theory. However, to specify the temperature dependence of the thermophysical characteristics, these physical qualities can be expressed as a constant value, a temperature-dependent function, or a User-Defined Function (UDF) that can be written in a particular computer language. Density and viscosity, two thermo-physical characteristics of PCMs, can occasionally be considered temperature-dependent and governed by certain correlations,

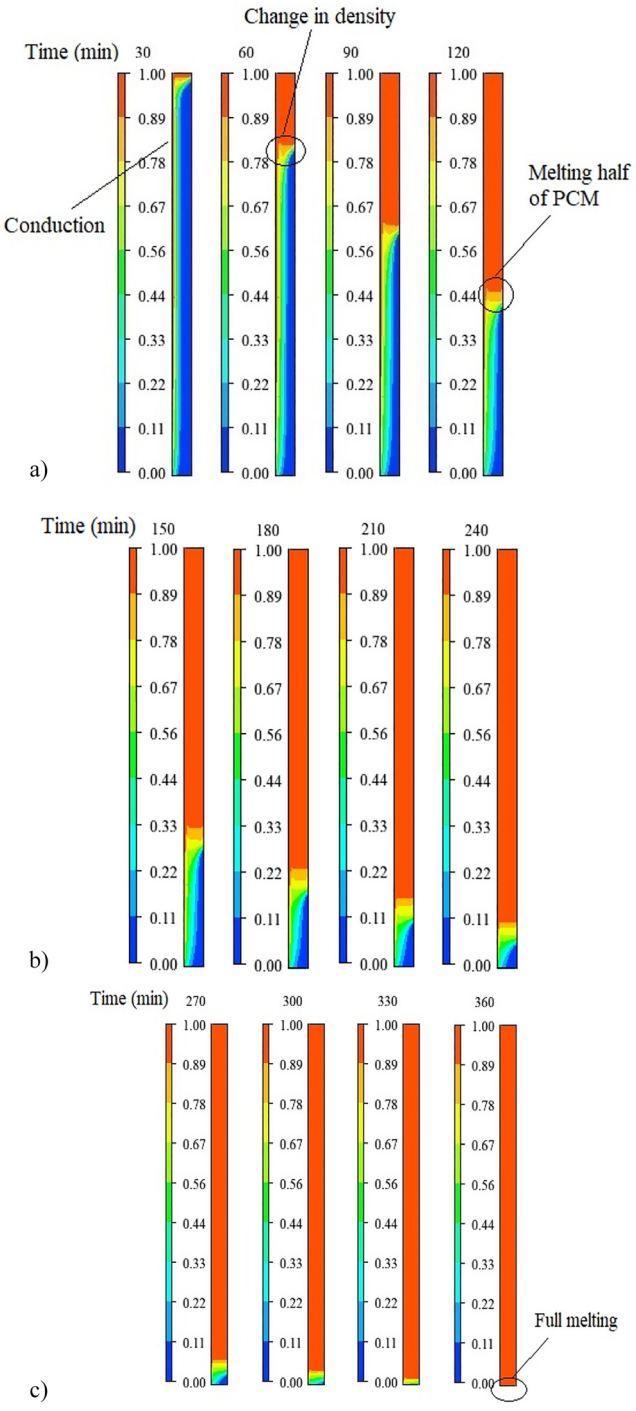

Fig. 5. Changes in liquid-fraction contours, a) Change in liquid-fraction (0–120 min), b) Change in liquid-fraction (150–240 min), c) Change in liquid-fraction (270–360 min) (*Source*: Authors')

$$\rho = \frac{\rho_1}{\beta(T - T_1) + 1}, \tag{7}$$

$$\mu = \exp\left(\frac{A + B}{T}\right), \tag{8}$$

where ρ_1 [kg m^{-3}] is the density of PCM at the melting temperature T_1; β is the thermal expansion coefficient; A, B are constant coefficients.

5. NUMERICAL RESULTS

The main goal of this paragraph is a summary of the numeric study of the melting process of phase change materials for the implementation of thermal storage systems in building envelopes. The numerical study of paraffin wax melting in a 10×200 mm rectangular zone is heated by convection from the left and right and adiabatically from the other two sides. The data were collected at 30 min intervals over the whole simulation's 360 min melting cycle. The change in a liquid fraction over time is seen in Fig. 5. It is clear how the melting interface moves and changes shape as time goes on. When a substance is entirely liquid ($f = 1$), and when it is entirely solid ($f = 0$). The melting front, which separates the liquid from the solid region, is represented by the mushy zone. For the first 30 min of the melting process, the melting interface is virtually parallel to the left wall, demonstrating that conduction is the main means of heat transfer at this time. The liquid PCM rises and falls repeatedly after 60 min has passed due to its lower density and higher temperature. Another thing to note is that the PCM chamber's top layer takes around 60 min to melt. In the following 90 min, around half of the PCM in the PCM chamber melts.

6. CONCLUSION

The paper comprehensively categorizes PCMs utilized in thermal energy storage technologies. The purpose was to highlight CFD as a useful technique for advancing the engineering of thermal energy storage systems. Because of the extremely exact findings, applying CFD to constructing PCM thermal storages is a method that may be used. In order to assist customers, save time and money and work as efficiently as possible, CFD also offers optimization tools.

According to numerical modeling and simulation of the PCM melting process under convection heat settings, heat transport happens mostly through conduction during the first 0–30 min of melting before switching to natural convection with more heating. The melting rate increases with time. As the melting process progresses, it grows in the middle and at the conclusion, although initially the same. In order to prevent convergence errors during the solution, the melting issue must be modeled using ANSYS (Fluent) with the appropriate meshing and time step selection.

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