NUMERICAL SIMULATION OF THERMAL ENERGY STORAGE SYSTEM USING PHASE CHANGE MATERIAL FOR FREE COOLING OF BUILDINGS

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ABSTRACT
A numerical investigation is adopted for a two dimensional thermal energy storage system (TES), employing finite element method to compute the time of charging or discharging energy from a phase change material (PCM) during day or night to utilize it in free cooling of space applying Baghdad Summer climate conditions (ambient temperature). A computer program is developed to analyze the thermal energy unit for different tube diameters, air flow rates and inlet air temperature for both solidification and melting processes. This study shows that utilizing small tube diameter, low flow rates or air inlet temperature near the fusion temperature lead to increase time of phase change process. It was also shown that the time duration of melting is larger than solidification.

Keywords: Free Cooling, PCM, Melting, Solidification, FEM.

INTRODUCTION
Phase change storage systems have been developed for many applications such as ice storage, conservation and transport of temperature sensitive materials, building insulation applications, etc. Employing the heat released or absorbed at melting/solidification temperature of phase change material (PCM) in space heating or cooling is an important feature of this process. A review of thermal energy storage particularly on moving boundary problems in different heat exchanger constructions is presented by Zalba et. al.(2003). A storage unit composed of spherical capsules filled with (PCM) placed inside a cylindrical tank is investigated numerically and experimentally by Ismail and Heriqniez (2002). They treated the solidification process using only one dimensional heat conduction employing finite difference approximation and a moving grid inside the spherical capsules. Zukowski (2007) analyze the heat and mass transferred in a ventilation duct filled with encapsulated paraffin wax (RII56) for short term heating by adapting three dimensional fully implicit (FDM).
The objective of the present work is to design and to analyze the thermal behavior of energy storage system shown in Fig.(1), utilizing (PCM) of melting temperature around (29.5°C), in order to employ it in a free cooling of a building by releasing heat during night and absorbing heat during day. Such application is feasible in climates where the temperature difference between day and night in summer is about (15°C).

MATHEMATICAL MODEL

Assumptions
To establish a convenient mathematical model to analyze the transient temperatures and heat transfer rates, the following assumptions have been introduced:

- The PCM is homogenous and isotropic and the thermo physical properties of solid phase are different from that of liquid phase.
- The thermo physical properties of PCM are independent on temperature.
- Thermal losses from system external boundary and radiation heat transfer inside the system are ignored.
- Forced convection fully developed air flow inside tubes.
- The initial temperature of the (PCM) is uniform and assumed at melting temperature \( T_m \) for solidification process, and at solidifying temperature \( T_s \) for melting process.

Governing Equation
The energy equation for a material undergoing a phase transformation is given as:

\[
\rho \frac{\partial H}{\partial t} + \rho \mathbf{u} \nabla H = k \nabla^2 T + s
\]  

For constant thermo physical properties (constant density) of the PCM and no heat sources, eq.(1) can be reduced to:

\[
\rho \frac{\partial H}{\partial t} = k \nabla^2 T
\]  

Substituting the left hand side by \( \rho c_p \frac{\partial T}{\partial t} \), yields:

\[
\rho c_p \frac{\partial T}{\partial t} = k \nabla^2 T
\]  

Geometry and Boundary Conditions
The initial condition specifies a constant temperature field at \( T_o \) at time zero. The boundary conditions, given as:

\[
\frac{\partial T}{\partial n} = 0
\]

at external boundary and plane of symmetry as shown in fig.(1), while that at internal surface of tube wall:
\[ k \frac{\partial T}{\partial n} = h_i(T - T_\infty) \]  

The internal heat transfer coefficient \( h_i \) is calculated for turbulent fluid flow according to (Kays and Crawford 1993) 

\[ h_i = \frac{k}{D} \left( \frac{(Re-1000) \cdot C_f / 2}{1 + 12.7 \sqrt{C_f / 2} \cdot (Pr^{2/3} - 1)} \right) \]  

\[ C_f = 2(2.236 \ln(Re) - 4.639)^2 \]  

Where \( C_f \) is Petukhov's friction coefficient for turbulent flow (Kays and Crawford 1993).

**NUMERICAL ANALYSIS**

Differential eq.(3) with initial and boundary conditions (eq.s (4) and (5) respectively), have been discretized using finite element method, employing Galerkin procedure leads to the following typical components of elemental mass and stiffness matrices \( (M^e \text{ and } K^e \text{ respectively}) \), and force vector \( F^e \) which can be defined as: 

\[ M^e_{jk} = \int_{\Omega^e} \rho C_p N_j N_k d\Omega^e \]  

\[ K^e_{jk} = \int_{\Omega^e} \nabla N_k \bullet (k \nabla N_j) d\Omega^e + \int_{\Gamma^e} h_i N_j N_k d\Gamma^e \]  

\[ F^e_k = \int_{\Gamma^e} h_i N_k d\Gamma^e \]  

The thermophysical properties during phase change process (solidification or melting) are calculated as: (using table (1))

\[ C_p = \frac{LH}{(T_m - T_s)} \]  

\[ k = F_s k_s + (1-F_s) k_m \]  

\[ \rho = F_s \rho_s + (1-F_s) \rho_m \]  

Where the subscripts \( (s) \text{ and } (m) \) refer to solid phase and melted phase respectively, and the elemental solid fraction is calculated using linear interpolation as:

\[ F_s = \frac{T - T_s}{T_m - T_s} \]  

where \( T \) refers to the elemental average temperature.

The elemental matrices and vector \( (M^e, K^e \text{ and } F^e) \)are assembled into global matrices and global vector to obtain a system of first order time dependent differential equation.
A recursive algorithm based on time marching technique (finite difference method) is adopted to solve eq.(15) (Smith and Griffiths 2004), so introducing a linear interpolation and fixed time step $\Delta t$:

$$T = \theta T^n + (1-\theta) T^o$$  \hspace{1cm} (16)$$

Where

$T^n$ and $T^o$ : new and old temperature values respectively

$\theta$ : constant such that $0 \leq \theta \leq 1$ (taking $\theta = 2/3$ based on Galerkin approach with unconditional stability)

Substituting eq.(16) in eq.(15) leading to the following result

$$[M + \theta \Delta t K] T^n = [M - (1-\theta) \Delta t K] T^o + \Delta t F$$  \hspace{1cm} (17)$$

Rearranging this equation to get a system of algebraic equations as:

$$[A] T^n = \{B\}$$  \hspace{1cm} (18)$$

Grid Generation

The mesh shown in fig.(1) represents a symmetrical quarter of thermal energy storage unit composed of (209) nodes and (180) quadrilateral linear four nodded elements. The first layer of elements adjacent to fluid represents the copper tube wall while the rest belong to PCM.

Computational Procedure

The computational steps followed in the present work are:

1- Read input data :
   a. Thermophysical properties of copper tube and of calcium chloride hexhydrate (PCM chosen in the present work is a hydrate salt) (Table (1)).
   b. TES unit size and tube diameter (Table (2)).
   c. Initial temperature
   d. Air inlet temperature, and flow rate.
   e. Time step.

2- Generate nodes coordinates and elemental nodes (local and global) and compute elemental area.

3- At each time step
   a. Increment time
   b. Form elemental matrices and vector
   c. Assemble elemental matrices and vector to global system
   d. Modify system matrices to form matrix $A$ and vector $B$
   e. Solve the system of simultaneous equations [eq.(18)] to evaluate $T^n$ using Gauss Elimination method for symmetrical matrix $A$

4- Proceed to the next time step

Time required to complete phase change (solidification or melting duration) can be determined by subtracting the time required to change the phase of the first node ($t_1$) from that required for the last node ($t_2$) in the analyzed domain.
a Fortran computer program is developed for the computational approach using (Fortran power station 95 software). The execution time varies between (7-10 min for time step of (10 s) depending on period of examination) on a personal computer Pentium 4.

RESULTS AND DISCUSSION

Verification of the Computer Program

The validity of the computational procedure and the computer program developed is examined by solving a two dimensional phase change problem which is initially at material fusion temperature \( T_f \) then suddenly subjected to \( T_1 \) in order to solidify the material as shown in fig.(2a). The results obtained are compared with that published by [Crowley 1978]. Fig.(2b) shows a good agreement between the computational and published results with maximum variation of 0.1%.

Solidification Process

Figures (3 to 5) indicate the transient temperature profile at a selected node of PCM (namely node 20) during solidification process. Fig(3) shows that the solidification duration decreases as the air flow rate increases, since increasing air flow rate causes an increase in Reynolds number, hence increasing heat transfer coefficient \( h_1 \) according to equation (6) for the same (PCM volume) value of thermal energy storage unit, thence increasing the heat transferred from air to PCM and decreasing solidification duration.

It is also shown that employing larger tube diameter leads to increase the surface area through which heat is transferred from air to (PCM), hence decreasing solidification time with fixed air inlet temperature and flow rate as shown in Fig. (4).

The effect of temperature difference between melting temperature of (PCM) (=29.9 \( ^\circ \text{C} \) in the present work) and air inlet temperature on solidification time can be shown in Fig.(5). It is clear that increasing the temperature difference leads to increase the heat transferred to air for the same flow rate and tube diameter, hence decreasing the solidification time.

Fig.(6) shows that the variation of air flow rate has no significant effect on solidification time for large tube diameters. While it has a considerable effect for small tube diameters, since for the same flow rates the air velocity is higher in small diameter which causes flow of high Reynolds number that affect the heat transfer coefficient \( h_1 \) as it is clear from eq.(6). It can also be deduced from this figure that air inlet temperature has a weak effect on solidification duration for a unit of large tube diameters while its effect is obvious for units of small tube diameters.

Fig.(7) shows that maximum energy exchanged between air and (PCM) for small tube diameters with high flow rate values while the minimum is for large tube diameter with low flow rate values.

Melting Process

Fig.(8) Shows the melting process during day for air inlet temperature and flow rate of (45 \( ^\circ \text{C} \) 150 \( \text{m}^3/\text{hr} \) respectively). It obviously shown that duration time of melting process during day is larger than that of solidification process during night. The factors affect melting process are air flow rate as indicated by Fig.(9), and tube diameter as shown in Fig. (10), while air inlet temperature has no significant effect on
melting time for all tube diameters investigated as shown in Fig. (10). This is due to the effect of these parameters on heat transfer coefficient.

CONCLUSION
An application of (PCM) in free cooling system is presented. Numerical experiments are conducted to specify the main parameters influence the thermal behavior of this system. The following concluding remarks can be drawn during this work as follows:

1- The solidification process is faster with:
   a- Increasing air flow rate
   b- Employing larger tube diameter
   c- Increasing the difference between inlet air temperature and melting temperature of PCM

2- A small effect for the air flow rate through large tube diameter on solidification time has been indicated while a significant effect for a unit with small tube diameter.

3- The variation of air inlet temperature has significant effect on solidification time for a unit with small tube diameter.

4- The most effective parameters on melting process are air flow rate and tube diameter of thermal energy storage unit.

REFERENCES:


NOMENCLATURE:
D    : Tube diameter (m)
\{F\} : Global force vector
$k$ : Fluid thermal conductivity (W/m°C)

$[K]$ : Global stiffness matrix

$[M]$ : Global mass matrix

$n$ : Unit normal vector

$Q$ : Air volumetric flow rate (m³/hr)

$Re$ : Reynolds number

$Pr$ : Prandtl number

$t$ : Time (s)

$T$ : PCM or tube wall temperature (°C)

$T_{in}$ : Air inlet temperature (°C)

$T_{\infty}$ : Air bulk temperature (°C)

$u$ : Velocity (m/s)

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Table (1): Thermo physical Properties of PCM (CaCl$_2$H$_2$O) (Zalba et al., 2003) and Copper Tube (Holman 1981)

<table>
<thead>
<tr>
<th>Property</th>
<th>Solid phase</th>
<th>Liquid phase</th>
<th>copper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity $k$</td>
<td>(W/m°C)</td>
<td>1.09</td>
<td>0.53</td>
</tr>
<tr>
<td>Specific heat $C_p$</td>
<td>(kJ/kg.K)</td>
<td>1.4</td>
<td>2.2</td>
</tr>
<tr>
<td>Density</td>
<td>(kg/m³)</td>
<td>1710</td>
<td>1530</td>
</tr>
</tbody>
</table>

Melting temperature $T_m = 29.9$ °C

Solidifying temperature $T_s = 29.5$ °C

Latent heat of fusion $LH = 187$ kJ/kg

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Table (2): TES unit Dimensions

<table>
<thead>
<tr>
<th>Tube Diameter (mm)</th>
<th>TES unit size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Height (H) (mm)</td>
</tr>
<tr>
<td>10</td>
<td>81.15</td>
</tr>
<tr>
<td>25</td>
<td>85.274</td>
</tr>
<tr>
<td>50</td>
<td>100</td>
</tr>
</tbody>
</table>
Fig. (1): (a) Thermal Energy Storage System, (b) Grid Generation of Quarter of Thermal Energy Storage Unit
Solid fraction = solid volume / (total volume)

\[ t = \frac{\alpha \text{(time)}}{L^2} \]

dimensionless time

\( \alpha \): thermal diffusivity
Fig. (3): Effect of Air Flow Rate on Solidification Time for TES of Tube Diameter $D=10$ mm, $T_{in}=25$ $^\circ$C (Temperature history at node 20)

Fig. (4): Effect of Tube Diameter on Solidification Time for Air Flow Rate =150 m$^3$/hr, $T_{in}=25$ $^\circ$C, (Temperature profile at node 20)
Fig.(5): Effect of Air Inlet Temperature on Solidification Time for Air flow rate =150 m$^3$/hr and Tube Diameter = 10 mm, (Temperature profile at node 20)

Fig.(6): Parameterization of Flow rate, Tube Diameter and inlet Temperature on Time of Solidification Process
Fig. (7): Parameterization of Flow rate, Tube Diameter and Inlet Temperature on energy exchanged during Solidification Process

Fig. (8): Time Duration of Solidification and Melting for \( Q = 150\text{m}^3/\text{hr}, D=50\text{ mm at node 20} \)
Fig.(9): Effect of Air Flow Rate on Duration Time of Melting for 
(D=10 mm, T_in=45°C)

Fig.(10): Parameterization of Flow rate, Tube Diameter and Inlet Air Temperature on 
Melting Duration