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Numerical investigation of the "PCM type and position influence" on the melting process in a concrete wall

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Abstract—The main aim of the paper is to investigate the influence of PCM type on the transition melting interface where the PCM loses its ability to completely melt within a concrete wall, and to locate the thermophysical properties of phase change material that has a direct effect on its position. In this work a comparative analysis was used on different type of PCM through a two-dimensional mathematical model for simulating and analyzing the melting and solidification of PCM in order to enhance and optimize its latent heat storage. The thermal performance and influence are evaluated using different PCM position for different PCM type with different thermophysical properties. The governing equation for energy transport were developed by the enthalpy method and discretized with volume control scheme which were solved iteratively using TDMA algorithm.

Keywords; Phase change material, Concrete, Thermal control.

I. INTRODUCTION

Since the second half of twentieth century, phase change material has become one of the most interesting research subjects. At first, some testing was done using PCM wall board and PCM concrete systems to enhance the thermal energy storage [1-3]. Reference [4] studied building-integrated phase change material. Parametric simulations of the thermal performance of the wall were performed to account for the influences of external and internal ambient environments, daily solar radiation, and thickness as well as the melting point of the PCM layer. The results show that, incorporating the appropriate phase change material layer can improve the thermal performances of the wall. Reference [5] developed an enhanced wall that reduces peak air-conditioning demand in residential area. Reference [6] have analyzed a north wall made with hydrate salt phase change material thermal performance as a storage medium in east-west oriented green house. Reference [7] has incorporated a one-dimensional mathematical model in order to analyze the latent heat storage wall.

II. MATHEMATICAL MODEL

Fig. 1 shows the physical system studied in the present work. It consists of a three layered composite PCM/concrete

wall, the middle layer is the PCM, located at a variable position x_m with a thickness of e_m =4cm the total thickness of the wall is L=20cm, the PCM type and its thermophysical properties are shown in table 1. the composite PCM wall is under influence of ambient air convection. In order to write the equation governing the physical model, it is necessary to perform a number of assumptions:

- The thermophysical properties are constant. Although different in the liquid and solid phases, it is assumed that densities, thermal capacities and thermal conductivities remain constant and independent of temperature.
- The horizontal boundaries are supposed to be adiabatic.
- The phase change is isothermal.
- Induced flow in the melted PCM because of the liquid velocity is negligible.



Figure 1: Physical model Imposed on different PCM

Or: $x_m = 1, x_m = 2, x_m = 3, x_m = 4, x_m = 5$

Material		T _m (℃)	$\Delta h_f(kj/kg)$	C _p (<i>KJ/kg</i> .℃)	$\rho(\text{kg}/m^3)$	k(w/m ² .K)
Salt hydrate S27 (inorganic)	S	25	175.0	2.2	1530	0.54
	L	25	175.0	2.2	1530	0.54
Organic PCM solution A25	S	25	150	2.15	785	0.18
	L	25	150	2.15	785	0.18
Polyglycol E600 (organic)	S	22	127.2	1.934	1126	0.358
	L	22	127.2	2.196	1232	0.148

Table 1:Thermophysical properties

The energy equation in its most general form contains a lot of variables. For a steady low velocity flow with negligible viscous dissipation, the energy can be written as:

$$div(\vec{\phi}) + \rho c_p \frac{\partial T}{\partial t} - p = 0$$
 (1)

Or $\vec{\phi} = -k \ \vec{grad}(T)$ and without any heat source for the concrete layer the equation (1) become:

$$\rho c_{p} \frac{\partial T}{\partial t} = \operatorname{div}(k \operatorname{grad}(T))$$
(2)

$$\rho c_{p} \frac{\partial T}{\partial t} = \nabla (k \nabla T)$$
(3)

As for the concrete a solid material we can write:

$$\rho c_{p} \frac{\partial T}{\partial t} = \frac{\partial h(T)}{\partial t}$$
(4)

For the phase change materials layer, we have a source term p which is the latent heat stored in the melting processes so the equation in PCM layer is:

$$\rho c_{p} \frac{\partial T}{\partial t} = \nabla (k \nabla T) + \frac{\partial (\rho \Delta h_{f} f + h(T_{m}))}{\partial t}$$
(5)

With:

$$p = \frac{\partial(\rho \Delta h_f f + h(T_m))}{\partial t}$$
(6)

Or:

$$\frac{\partial H(T)}{\partial t} = \frac{\partial h(T_m)}{\partial t} + \rho c_p \frac{\partial T}{\partial t} + \rho \Delta h_f \frac{\partial f}{\partial t}$$
(7)

To make the equation more adaptable and compatible for a numerical discretization we combined all the seen equation for every layer into one:

$$\frac{\partial H}{\partial t} = \nabla(k \ \nabla T) \tag{8}$$

With:
$$\begin{cases} H(T)=h(T)+\rho \Delta f \rho \Delta h_f \\ h(T)=h(T_m)+\int_{T_m}^T \rho c_p dT \end{cases}$$
(9)

 λ is introduced to make the equation more flexible so that we use one formula for both the concrete layers ($\lambda=0$), and PCM layer ($\lambda=0$).

With the use of sensible enthalpy, eq (8) is rewritten:

$$\nabla(\mathbf{k}\,\nabla\mathbf{T}) = \frac{\partial\mathbf{h}(\mathbf{T}_{\mathrm{m}})}{\partial\mathbf{t}} + \rho\mathbf{c}_{\mathrm{p}}\frac{\partial\mathbf{T}}{\partial\mathbf{t}} + \rho\lambda\Delta\mathbf{h}_{\mathrm{f}}\frac{\partial\mathbf{f}}{\partial\mathbf{t}} \quad (10)$$

$$\nabla \left(\frac{\kappa}{\rho c_p} \nabla h(t) \right) = \rho c_p \frac{\partial I}{\partial t} + \rho \lambda \Delta h_f \frac{\partial I}{\partial t}$$
(11)

Or the thermal diffusivity $\alpha = \frac{k}{\rho c_p}$.

$$\frac{\partial \mathbf{h}(\mathbf{T})}{\partial \mathbf{t}} = \alpha \frac{\partial^2 \mathbf{h}(\mathbf{T})}{\partial \mathbf{x}^2} + \alpha \frac{\partial^2 \mathbf{h}(\mathbf{T})}{\partial \mathbf{y}^2} - \rho \lambda \Delta \mathbf{h}_f \frac{\partial \mathbf{f}}{\partial \mathbf{t}}$$
(12)

The liquid fraction f is estimated as:

$$f = \begin{cases} 1 \text{ if } T > T_m \\ 0 \text{ if } T < T_m \\ 0 < f < 1 \text{ if } T = T_m \end{cases}$$
(13)

Thanks to the continuity of temperature and heat flux density at the interfaces concrete/PCM $\mathbf{k}_{+\frac{\partial T}{\partial x}}\Big|_{x_{+}} = \mathbf{k}_{-\frac{\partial T}{\partial x}}\Big|_{x}$, $\mathbf{T}_{+} = \mathbf{T}_{-}$ we can obtain the thermal properties of the interfaces by the following formulas:

$$k_{i} = \frac{k_{+}k_{-}(\delta_{-} + \delta_{+})}{k_{+}\delta_{-} + k_{-}\delta_{+}}$$
(14)

$$\mathbf{k}_{\mathrm{m}} = \mathbf{f} \mathbf{k}_{\mathrm{l}} + (1 - \mathbf{f}) \mathbf{k}_{\mathrm{s}}$$
(15)

$$\rho c_p = f(\rho c_p)_1 + (1-f)(\rho c_p)_s$$
(16)

 δ_{-} , δ_{+} are the distance between the first node inside the PCM region and the first one inside the concrete layer.

III. INITIAL AND SURFACE CONDITIONS

At the moment t=0, the different layers of the wall have the same initial temperature $T_{Ini}=18$ °C.Surface conditions reflect the coupling between the different layers at the interfaces level. and for the external convective variables are imposed during 24 hours.

- At x=0 (Internal wall) $k \frac{\partial T}{\partial t}\Big|_{x=0} = h_i(T_c - T)$ (17)
- At **x=L** (external wall)

$$\left. k \frac{\partial T}{\partial t} \right|_{x=L} = h_a(T_a - T)$$
(18)

- Heat flux at the interfaces, at x=x_m and x=x_m+e_m, between the PCM layer and the concrete

$$q_{i}^{"} = \frac{k_{+}k_{-}}{k_{+}\delta_{-}+k_{-}\delta_{+}}; T_{+}=T_{-}$$
 (19)

IV. NUMERICAL SCHEME

The obtained nonlinear equations are integrated on a uniform mesh to discretize it using the finite volume method. We focus on the grid point P that is shown in Fig. 2 a portion of a two-dimensional grid. Point E and W are its x-direction neighbors, while points N and S are the y-direction neighbors. The control volume around P is shown by dashed lines.



Figure 2 : Control volume for the two-dimensional situation

To obtain the finite difference equation, the eq (12) is integrated over each control volume.

$$\int_{y_s}^{y_n} \int_{x_w}^{x_e} \frac{\partial h(T)}{\partial t} dx dy = \int_{y_s}^{y_n} \int_{x_w}^{x_e} \alpha \frac{\partial^2 h(T)}{\partial x^2} dx dy + \int_{y_s}^{y_n} \int_{x_w}^{x_e} \alpha \frac{\partial^2 h(T)}{\partial y^2} dx dy - \int_{y_s}^{y_n} \int_{x_w}^{x_e} \rho \lambda \Delta h_f \frac{\partial f}{\partial t} dx dy$$
(21)

$$\int_{y_{e}}^{y_{n}} \int_{x_{w}}^{x_{e}} \frac{\partial h(T)}{\partial t} dx dy = \frac{h_{p}^{t} - h_{p}^{o}}{\Delta t} \Delta x \Delta y$$
(22)

$$\int_{y_{c}}^{y_{n}} \int_{x_{w}}^{x_{e}} \alpha \frac{\partial^{2} h(T)}{\partial x^{2}} dx dy = \left[\alpha \frac{\partial h(T)}{\partial x} \Big|_{e} - \alpha \frac{\partial h(T)}{\partial x} \Big|_{w} \right] \Delta y \qquad (23)$$

$$\int_{y_{c}}^{y_{n}} \int_{x_{w}}^{x_{c}} \alpha \frac{\partial^{2} h(T)}{\partial y^{2}} dx dy = \left[\alpha \frac{\partial h(T)}{\partial y} \Big|_{n} - \alpha \frac{\partial h(T)}{\partial y} \Big|_{s} \right] \Delta x \qquad (24)$$

$$\int_{y_c}^{y_n} \int_{x_w}^{x_c} \rho \lambda \Delta \mathbf{h}_f \frac{\partial \mathbf{f}}{\partial t} d\mathbf{x} d\mathbf{y} = \rho \lambda \Delta \mathbf{h}_f (\mathbf{f}_p^t - \mathbf{f}_p^0) \Delta \mathbf{x} \Delta \mathbf{y}$$
(25)

With:

$$\alpha \frac{\partial h(T)}{\partial x} \Big|_{e} \Delta y = \alpha_{e} \frac{(h_{e} - h_{p})}{x_{e} - x_{p}} \Delta y ; (\delta x)_{e} = x_{e} - x_{p}$$
(26)

$$\alpha \frac{\partial h(T)}{\partial x} \Big|_{w} \Delta y = \alpha_{w} \frac{(h_{p} - h_{w})}{x_{p} - x_{w}} \Delta y ; \quad (\delta x)_{w} = x_{p} - x_{w} \quad (27)$$

$$\alpha \frac{\partial \mathbf{h}(\mathbf{T})}{\partial \mathbf{y}} \Big|_{\mathbf{n}} \Delta \mathbf{x} = \alpha_{\mathbf{n}} \frac{(\mathbf{h}_{\mathbf{n}} - \mathbf{h}_{\mathbf{p}})}{\mathbf{y}_{\mathbf{n}} - \mathbf{y}_{\mathbf{p}}} \Delta \mathbf{x} \quad ; \quad (\delta \mathbf{y})_{\mathbf{n}} = \mathbf{y}_{\mathbf{n}} - \mathbf{y}_{\mathbf{p}} \quad (28)$$

$$\left. \alpha \frac{\partial n(1)}{\partial y} \right|_{s} \Delta x = \alpha_{s} \frac{(n_{p} - n_{s})}{y_{p} - y_{s}} \Delta x ; (\delta y)_{s} = y_{p} - y_{s}$$
(29)

We can write the eq(21) as follow:

At last we can have the discretization equation for numerical calculation:

$$a_{p}h_{p}+a_{n}h_{n}+a_{s}h_{s}+a_{w}h_{w}+a_{e}h_{e}=b \qquad (30)$$

Where:

$$\begin{cases} a_{n} = \frac{\alpha_{n}\Delta t}{(\delta y)_{n}\Delta y} ; a_{s} = \frac{\alpha_{s}\Delta t}{(\delta y)_{s}\Delta y} \\ a_{e} = \frac{\alpha_{e}\Delta t}{(\delta x)_{a}\Delta x} ; a_{w} = \frac{\alpha_{w}\Delta t}{(\delta x)_{w}\Delta x} \\ \begin{cases} a_{p} = 1 - a_{n} - a_{s} - a_{e} - a_{w} \\ b = h_{p}^{0} + \rho\lambda\Delta h_{f}(f_{p}^{0} - f_{p}^{t}) \end{cases}$$
(31)

The equation is solved, step by step, using TDMA algorithm.

V. RESULT AND DISCUSSION

In order to assess the reaction of PCM position into the wall to the PCM type, the time wise evolution of the melting interface was evaluated, Fig 3. After almost 18 hours, the PCM is completely melted for the three PCM. for $x_m=1$, $x_m=2$, or $x_m=3$. Then they start to re-solidify until midnight.



Figure 3: melting interface of the three PCMs

As for the Organic PCM solution A25, and the Salt hydrate S27 (inorganic), at $x_m = 4$ and $x_m = 5$, Fig. 4 shows that the melting process does not happen.



Figure 4: melting interface of Organic PCM solution A25 and Salt hydrate S27.

Contrary to the two previous PCM, Polyglycol E600 simulation shows that it is completely melting at day and solidify until midnight at $x_m = 4$ and he lost its ability to melt at $x_m = 5$.

After taking a look at the simulation results of the Organic PCM solution A25, and the Salt hydrate S27 (inorganic) we observed that they lost their ability to melt at the same interface position even though they have the same melting temperature and different thermophysical properties. As for the Polyglycol E600 (organic) which has an inferior melting temperature it lost its ability to melt at a more advanced interface then the previous ones.

Those results confirm that there is a transition interface where the pcm lose its ability to melt, and that interface isn't influenced by the PCM type but by the difference between melting temperature of the PCM and the ambient temperature, the lower it gets the more the transition interface advance.

VI. CONCLUSION

A numerical code was developed using the finite volume method, to evaluate the liquid fraction behavior of PCM based on its type and position. The simulation was executed using three different PCM type that were placed in different position at the left side of the concrete wall. The system concrete/PCM was evaluated during 24 hours. Results showed that the PCM loses its ability to completely melt after reaching a transition interface, where its position depends on the PCM melting temperature.

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