# THERMAL CONDITIONING USING PHASE CHANGE MATERIALS

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## ABSTRACT

A combined procedure using a classical qualitative result for initial and boundary problems associated to parabolic equations, numerical treatment and computational simulation, have been used to obtain some results on the dynamic behavior of the function that provides the position of the melting interface or moving front of the phase change material at each time. This material is used in a special device that is designed in order to get thermal conditioning in physical - chemical systems of practical importance. A monotone dependence of the melting interface upon some parameters is also shown.

**Key words:** phase change materials, melting interface, thermal conditioning

## INTRODUCTION

The use of phase change materials in thermal conditioning presents different possibilities according to the place to be conditioned. They also have the advantage of reducing energy consumption (Abhat,1983).
In a passive solar system, phase change materials may be employed as substitutes for thermal mass. They have a high thermal storage capacity and a low weight and volume per unit of energy storage when compared with traditional materials in use (Handan and Elvers, 1996).
They may be incorporated in building materials like tiles, walls, or ceiling panels (Bouciguez, 1998). In other situations the thermal storage material may be incorporated in special containers into or along the wall or window structure (Charach and Zarni, 1987).
Once the operating temperature has been determined, the selection of a suitable phase change material can be made. The weight and volume of the amount of material required providing the needed storage capacity can now be determined. This, in turn, will provide the information needed for the structural design.
The phase change materials must meet proper performance requirements, be safe, have a reasonable life expectancy, and be available in proper quantities and at reasonable cost.
When placed in properly designed containers or modules, phase change materials should present no problems over their usable lifetime. The manufacturing and disposal of these materials will likewise not create environmental problems or introduce harmful materials into the environment.
We propose now the use of phase change materials, to keep the optimal temperature of conservation in the transport of agricultural products.
In fact, the agricultural products need special conditions on temperature and moisture during the stages of storage and transport. Phase change materials can be used in order to keep the required temperature.
Taking into account that generally, the external temperature that is applied to the phase change material is a non-monotone function of time and there is no restriction on its sign, a descriptive model taking into account such situation has been formulated.

## GENERAL CONSIDERATIONS

*Phase change material selection*
There are many suitable materials available. However, the materials used in a given application have to be carefully chosen to match the need. In general, a phase change storage material must meet the following requirements:

- phase change at the appropriate temperature.
- safety and compatibility with applicable codes and standards
- reliability over a reasonable life cycle
- availability and independence of scarce energy supplies
- reasonable cost

In particular, organic compounds, in contrast to inorganic ones, do not show super cooling and they are more stable than the inorganic ones (Hasan and Sayigh, 1994).
Organic materials, specially wax-like substances, such as the esters of fatty acids have been recommended for heat storage. Their heat of fusion, density, thermal conductivity and specific heat are around 120 kJ/kg, 800 kg/m$^3$, 0.20 W/m C and 1500 J/kg C, respectively (Suvern, 1994).
Phase change materials have a significant potential in many situations where the applications of thermal storage are otherwise out of the question due to space and/or weight limitations.

*Physical and chemical aspects*

In order to assure a good performance, the phase change materials should present the following physical and chemical properties to be used in thermal conditioning

- a defined point of fusion
- a melting point in the desired operating temperature range
- high latent heat of fusion per unit mass
- high specific heat
- constant density in the operation temperature range
- its density in the liquid and solid phase must be similar
- its liquid and solid phase must have identical composition
- chemical stability and no chemical decomposition
- no corrosible, no flammable, no toxic, no explosive
- no super cooling problem

## MODEL FORMULATION

*Preliminaries*

The following general conditions are assumed:

a) Both, materials and heat transfer parameters for the phase change substances are constant along the whole process

b) The Fourier's law holds for the one dimensional heat conduction.

*Descriptive Model*

Taking into account the former considerations, the following initial and free boundary problem (Stefan's problem) must be satisfied by the temperature profile *u(x,t)* and the function *s(t)*

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \qquad \forall t > 0, \qquad 0 < x < s(t) \le e \tag{1}$$

$$u(s(t),t) = 0, \quad \forall t > 0 \tag{2}$$

$$\rho L \frac{ds(t)}{dt} = -k \frac{\partial u(x = s(t))}{\partial x}, \qquad \forall t > 0 \tag{3}$$

$$u(x,0) = 0, \qquad o < x \le e \tag{4}$$

$$u(0,t) = g(t) \quad \forall t > 0 \tag{5}$$

$$s(0) = 0 \tag{6}$$

Where it is important to recall that the boundary temperature data *g(t)* is assumed to be a non-monotone continuous function without restriction in its sign. Figure 1 presents the scheme of the modeling phase change material, showing its dimensions.

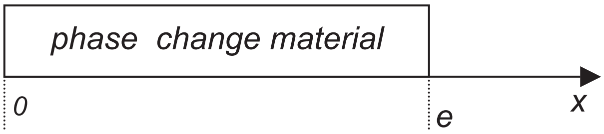

Figure 1. Scheme of the considered geometry for the phase change material.

## QUALITATIVE RESULTS ON THE MODEL SOLUTION

*Dynamic Behavior of the Melting Interface Position s(t)*

Let *u=u(x,t)*, *s=s(t)* be a solution for the model (1) - (6) and let *g=g(t)* be a boundary data such that:

$$g(t) > 0, \qquad \forall t \in (0, t_0), \qquad g(t_0) = 0; .. \qquad g(t) < 0, \ . \ \forall t \in (t_0, t_0 + \varepsilon), \quad \varepsilon > 0, \tag{7}$$

Then *s(t)* is a non-increasing function $\forall t \quad (t_0,t_0+ \quad )$. In fact, by contradiction let us suppose the following behavior for *s(t)*: *s(t)* is a monotone increasing function $\forall t \quad (t_0,t_0+ \quad )$.

Let $t^* \quad (t_0,t_0+ \quad )$. Since $u(s(t^*),t^*)=0$, there exists a left neighborhood of $(s(t^*),t^*)$ where $u>0$ and there exists a right neighborhood of $(x=0,t_0)$ where $u<0$. Hence, it follows that there exists a local maximum for the temperature profile *u(x,t)* for $x \quad (0,s(t^*))$. The occurrence of such local maximum is not possible in virtue of the weak maximum principle for parabolic equations.

*Simulation results*

In order to obtain the numerical solution, the descriptive model given by Eqs. (1) - (6), was applied for a general substance, with their parameters in the order of those for pure organic materials. An application with real material has been done too. Lauric aldheide and paraffin have been the choice because they have different thermal parameters and equal melting point.

The descriptive model given by Eqs. (1) - (6), was applied for the particular case of lauric aldheide and paraffin as phase change materials, in order to obtain the numerical solution.

For such particular free boundary problem all the assumptions that were explicated in the former sections, together with the conditions for temperature data g(t) given by Eq. (7), were used.

In the numerical treatment, an explicit finite difference scheme with QB was applied. Temperature *g=g(t)* and thermal parameters data, used in the numerical solution are shown in Tables 1 and 2 respectively.

Table 1. Temperature g(t) used in the simulation.

| *t* (hs) | *g(t)*(C) | *t* (hs) | *g(t)*(C) | *t* (hs) | *g(t)*(C) | *t* (hs) | *g(t)*(C) | *t* (hs) | *g(t)*(C) | *t* (hs) | *g(t)*(C) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.2 | 4 | 2.01 | 8 | 0.5 | 12 | 1 | 16 | 1.02 | 20 | 0.05 |
| 0.5 | 2.1 | 4.5 | 1.2 | 8.5 | 0 | 12.5 | 1.2 | 16.5 | 0.09 | 20.5 | 0.1 |
| 1 | 3.5 | 5 | 0 | 9 | -0.1 | 13 | 1.5 | 17 | 0.05 | 21 | 0.08 |
| 1.5 | 5 | 5.5 | -0.8 | 9.5 | -0.6 | 13.5 | 1.9 | 17.5 | 0 | 21.5 | 0.002 |
| 2 | 5.6 | 6 | -2.5 | 10 | -0.2 | 14 | 2.5 | 18 | -0.01 | 22 | 0.0001 |
| 2.5 | 3 | 6.5 | -1 | 10.5 | 0.01 | 14.5 | 3.2 | 18.5 | -0.8 | 22.5 | -0.2 |
| 3 | 4.9 | 7 | 0 | 11 | 0.5 | 15 | 1.5 | 19 | -0.5 | 23 | -0.1 |
| 3.5 | 2.8 | 7.5 | 0.1 | 11.5 | 0.8 | 15.5 | 1.1 | 19.5 | -0.1 | 23.5 | 0 |

Table 2. Thermal parameters of the substance used in the simulation.

| phase change material | k (W/ m C) | ρ ($kg/m^3$) | c (J/kg C) | L (J/kg) |
|---|---|---|---|---|
| generic material | 0.20 | 800 | 1500 | 120000 |
| lauric aldheide | 0.20 | 880 | 1600 | 120000 |
| paraffin | 0.14 | 770 | 2890 | 180000 |

In Figure 2, the solution curves for the melting interface *s(t)* in meters vs. time *t* in hours corresponding to the lauric aldheide and paraffin are presented. The same figure also shows the graph for the temperature boundary data *g(t)*.

From such figure, it can be seen that the melting interface *s=s(t)* shows a dynamic behavior such as it was theoretically predicted using the weak maximum principle for parabolic equations in heat conduction.

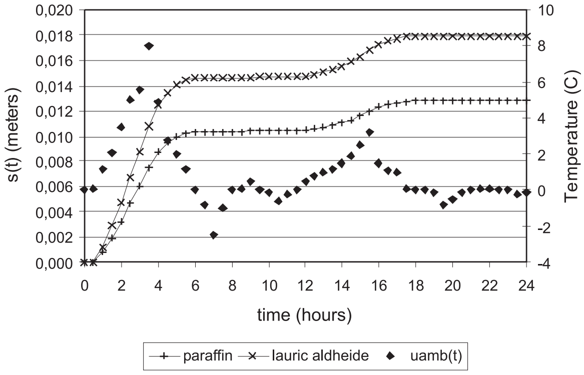

Figure 2. Numerical results for paraffin and lauric aldheide.

*Monotone dependence upon thermal and material parameters*

In order to evaluate the influence of different levels of parameters on the evolution of the melting interface *s=s(t)*, the model (1) - (6) was applied to a general phase change material having thermal and material parameters of the order of pure organic substances and was solved numerically.

As it can be seen in Figs. 3 to 5, showing the solution curves of the melting interface *s(t)* vs. time *t* and the graph of temperature data *g(t)*, a reasonable monotone dependence upon thermal conductivity, density and latent heat is exhibited.

The melting interface *s(t)* vs. time *t* and the graph of temperature data *g(t)* with different values of the specific heat is shown in figure 6. It can be seen that the variation of that parameter has no influence on the interface position.

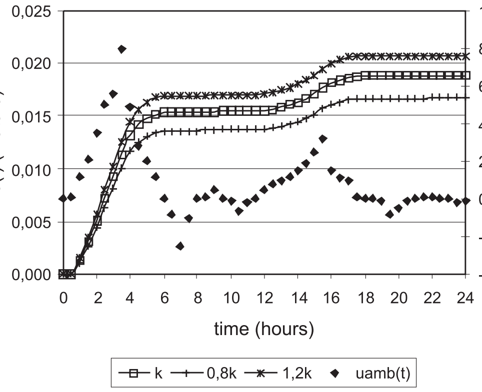

Figure 3. Dependence of the thermal conductivity.

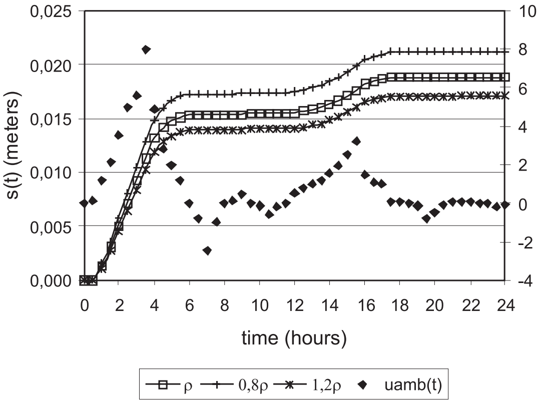

Figure 4. Dependence of the density.

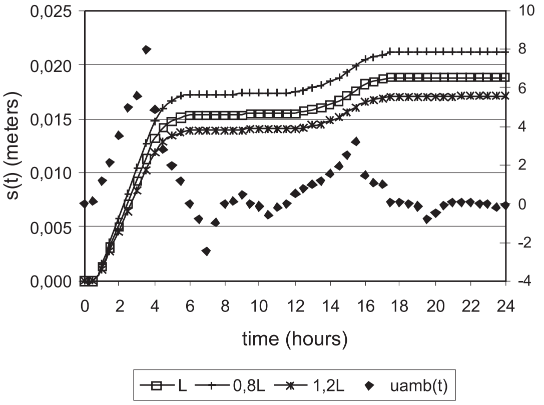

Figure 5. Dependence of the latent heat.

## CONCLUSIONS

A physical system, that presents a non-classical situation in heat conduction with phase change, was analyzed: the case of boundary temperature data being a non-monotone function of time without restriction on sign was studied.

It is important to recall that such particular situation may be of special interest for practical applications such as thermal conditioning. In fact, it is common that the boundary temperature data in the operating conditions of the system is in accordance with the case presented here. Regarding the melting interface, results on the dynamic behavior of a system when a general boundary temperature data is used and monotone dependence upon thermal and material parameters are presented.

From Figure 2, it can be seen that in the search for the phase change material to be used in a specific application, the melting point is a decisive factor. Moreover, thermal parameters also play an important role to assure an adequate heat transfer.

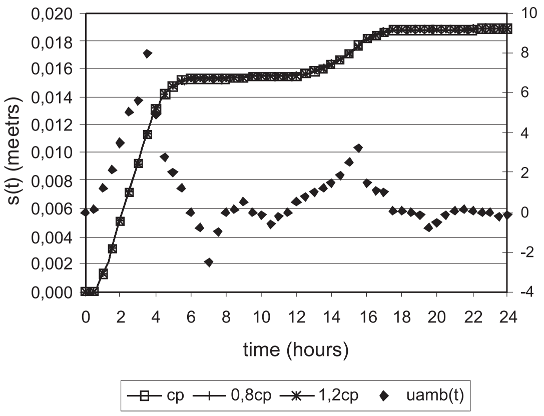

Figure 6. Dependence of the specific heat.

## NOMENCLATURE

| | |
|---|---|
| $x$ | spatial independent variable |
| $t$ | time independent variable |
| $T=T(x,t)$ | unknown function that denotes temperature profile of the phase change material |
| $s=s(t)$ | unknown function that denotes the position at time $t$ for the melting interface |
| $T_f$ | melting temperature |
| $f(t)$ | external boundary temperature |
| $g(t) = f(t) - T_f$ | difference between external boundary temperature and melting temperature |
| $u(x,t)=T(x,t) - T_f$ | difference between unknown temperature and melting temperature |
| $k$ | thermal conductivity of the phase change material |
| $c$ | specific heat of the phase change material |
| $L$ | latent heat of fusion of the phase change material |
| $e$ | width of the phase change material |
| $\rho$ | density of the phase change material |
| $\alpha=k/(\rho c)$ | thermal diffusivity |

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