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MODELING A FLAT PLATE PAINTED WITH PHASE CHANGE MATERIAL

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ABSTRACT

A model has been proposed for predicting the variation of heat capacity with temperature in composites containing a fraction of material that undergoes a phase change. Experimental data was collected for transient heat flux through a thin plate coated with a Phase Change Material (PCM). A finite difference routine was developed which implements the effective heat capacity model. The numerical solutions were compared to the experimental data to test the validity of the model.

NOMENCLATURE

c heat capacity (J/kg-C)
c_1 heat capacity, non-phase change region (J/kg-C)
F fraction of phase change material in mixture
Q non-dimensional heat rate
q rate of energy addition to sphere (W)
T temperature (C)
T_{pc} phase change temperature (C)
t time (sec)

α thermal diffusivity (m^2/sec)
α_1 thermal diffusivity, non-phase change (m^2/sec)
Δh heat of fusion (J/kg)
σ width of phase change region (C)(4° C)
σ_{eff} effective width of phase change region (C)
τ non-dimensional time
Θ non-dimensional temperature
$\Theta_{pc,eff}$ non-dimensional, effective phase change temp

INTRODUCTION

For mixtures that contain some fraction of phase change material, transient temperature measurements show a smearing of the expected level temperature response during the phase change. Theory predicts that when an object is heated, the temperature should increase until it reaches the phase change temperature. Upon reaching the phase change temperature, the temperature should remain constant while the object changes phase. After the phase change is complete, the temperature will resume increasing. In reality, the phase change process can be observed to influence temperature rise in the object over a range of temperatures near the phase change temperature. For example, Differential Scanning Calorimeter (DSC) plots for non-homogeneous mixtures show a smearing in energy absorption along with a shift away from the expected phase change temperature[1]. This behavior might be attributed to the fact that the measured temperatures represent the temperature of a region in space, not the temperature at a point.

If the measured temperature represents the temperature of a region in space, a heat capacity based on the average bulk temperature in a region will be more accurate for modeling phase change than a heat capacity based on the temperature at a point. For example, consider the heating of a sphere of phase change material surrounded by non-phase change material. The non-phase change material must be at a higher temperature than the phase change temperature before energy can be conducted into the phase change region of the sphere. At this same instant in time, the center of the sphere would be at a temperature lower than the phase change temperature. Thus temperatures both above and below the phase change temperature will exist while the material undergoes phase change. If observing the region as a whole, the phase change will occur over a wider range of temperature than expected.

Following this line of thought, Bowman and Brown[2] have proposed a method of modeling phase change that accounts for this behavior. They call it the "effective heat capacity" model. In their model, heat capacity is based

on average temperature of a mixture. The heat capacity function is shown to be dependent on temperature, percent phase change material in the mixture, and rate of energy addition. The model is useful when simulating mixtures where the phase change particles are small in comparison to the numerical grid used for the simulation. It is also useful in simulating experiments where temperature measurements represent regions larger than the phase change particles in the regions.

This paper describes a research effort to test the validity of the effective heat capacity model. Experiments were conducted with flat plates coated with paint containing microencapsulated phase change material. The effective heat capacity model was used in a numerical model to simulate the transients. The experimental and numerical data were compared.

HEAT CAPACITY MODEL

For the effective heat capacity model, the heat capacity is modeled using a normal distribution. The width of the phase change region is specified using the effective standard deviation (σ_{eff}) of the normal distribution. The phase change occurred in the vicinity of the effective phase change temperature ($T_{pc,eff}$). The area under the normal distribution is equal to the phase change energy. Heat capacity is assumed to be constant in the non-phase change portions of the transient. The heat capacity function used is:

$$c = c_1 + \frac{\Delta h}{\sigma_{eff}\sqrt{\pi}} \exp\left(-\frac{z^2}{2}\right) \qquad \text{Eq 1}$$

$$z = \frac{T - T_{pc,eff}}{\sigma} \qquad \text{Eq 2}$$

where c is the heat capacity, c_1 is a reference heat capacity (non-phase change value), and Δh is the heat of fusion. The effective phase change temperature and effective standard deviation are found from the expressions:[2]

$$\Theta_{pc,eff} = 0.027QF - 4.52F - 0.021Q + 4.34 \qquad \text{Eq 3}$$

$$\frac{\sigma_{eff}}{\sigma} = 0.0067QF - 4.52F - 0.010Q + 5.61 \qquad \text{Eq 4}$$

where $\Theta_{pc,eff}$ is the effective phase change temperature (non-dimensional), F is the fraction of phase change material in the mixture and σ_{eff} is the effective width of the phase change region .

$$\Theta_{pc,eff} = \frac{T_{pc,eff} - T_{pc}}{\sigma} \qquad \text{Eq 5}$$

$$Q = \frac{q}{r_o k \sigma} \qquad \text{Eq 6}$$

Where q is the rate of energy addition to the sphere, r_o is the sphere diameter, k is thermal conductivity and σ is the width of a non adjusted phase change region.

EXPERIMENTAL DATA

Six flat plates were tested. Each plate used a 3.0 mm thick carbon composite panel for the base material. Each panel was coated with a polyurethane coating on one side. The coating thickness varied for the different panels from 0.3 to 0.6 mm. Microencapsulated spheres of phase change material was added to the coating. Percent phase change material in the coating varied from 0% to 40%. The phase change material was Therasorb 143 (a Frisby Technologies trademark). The capsules were 10 to 40 microns in diameter. The material has a phase change temperature of 82.5 C, and the heat of fusion is 314 kJ/kg. A series of experiments were conducted to measure the properties of the flat plates. Table 1 contains the properties measured.

A transient was created by heating a plate from one side using a resistance heater located on top of the plate. The bottom side of the plate was cooled with a cold shoe. Heat flux gauges sandwiched on both sides of the plate measured the energy flux in to and out of the plate during the transients. Thermocouples were also located on both sides of the flat plate along with the heat flux gauges. For some of the tests, a third thermocouple was imbedded in the polyurethane coating. The heat flux and temperature sensors were used to document the thermal response of the flat plate to the energy addition from the heater. The entire system consisting of the heater, heat flux guages, thermocouples, test plate and cold shoe were clamped together to minimize variations in contact conductance from test to test. The temperature measurements were accurate to 1° K while the heat flux measurements had an uncertainty as high as 20%.

HEAT CAPACITY MODEL VALIDATION

To test the effective heat capacity model described above and presented in Eqs. 1 through 6, the experiments described above were simulated using the model. The one-dimensional heat diffusion equation was solved using finite difference methods. The experimental initial conditions along with the experimental energy fluxes in and out of the plate were used as the problem boundary conditions.

To model with confidence the case of a composite plane wall with heat flux on both sides, and temperature dependant c, we first worked with a number of simplified problems, which helped us gain confidence in our method. These preliminary tests included a homogeneous plane wall with constant temperature boundary conditions in one case and constant heat flux in another. Also studied was the case of a composite wall with given heat flux at the boundaries.

GOVERNING EQUATION

One-dimensional transient heat conduction is governed by the following equation:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) \qquad \text{Eq 7}$$

Although density changes may occur during phase changes in the material, these changes are relatively small and will be ignored in this study. The heat capacity model in this study, predicts that c will vary directly with temperature. We will see later that due to our discretization method, c will always by calculated from the temperature of a previous time-step, so that calculation of c will always be explicit. As there is no energy generated or lost, no source terms are present.

NUMERICAL METHOD

The discretization method used in this study follows the general form outlined by Patankar[4]. His general form is as follows:

$$\begin{aligned} a_P T_P = {} & a_E \left[f T_E + (1-f) T_E^0 \right] \\ & + a_W \left[f T_W + (1-f) T_W^0 \right] \\ & + \left[a_P^0 - (1-f) a_E - (1-f) a_W \right] T_P^0 \end{aligned} \qquad \text{Eq 8}$$

where:

$$a_E = \frac{k_e}{(\Delta x)_e} \qquad \text{Eq 9}$$

$$a_W = \frac{k_w}{(\Delta x)_w} \qquad \text{Eq 10}$$

$$a_P^0 = \frac{\rho c \Delta x}{\Delta t} \qquad \text{Eq 11}$$

$$a_P = f a_E + f a_W + a_P^0 \qquad \text{Eq 12}$$

Here, we will assume that the spacial grid is uniform, and that all control volume interfaces lie exactly midway between the grid points. All values or properties evaluated exactly at a grid-point are denoted by an upper-case subscript, while properties at control volume interfaces are denoted by lower case. The letter “P” is used to represent any given point, while “E” and “W” represent points to the left and right side of the point, respectively. The temporal grid is also uniform, and one time step is

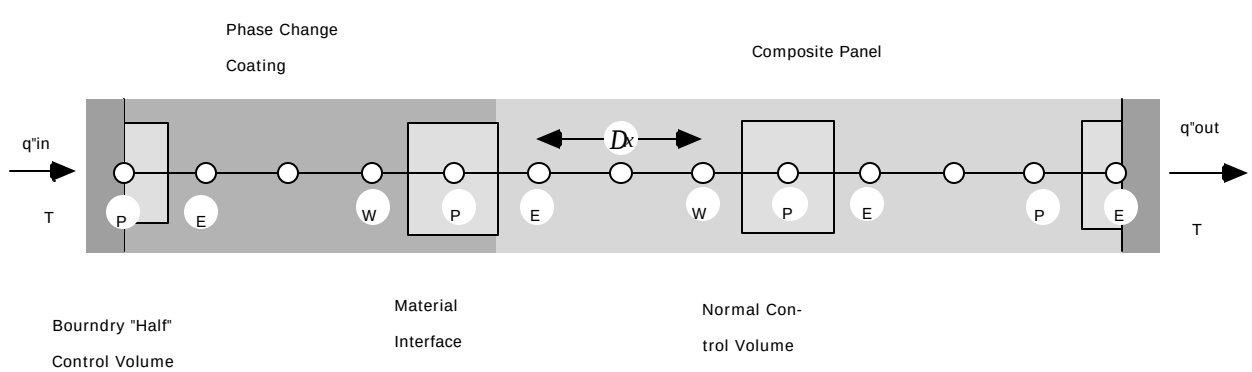

Figure 1 Simplified spacial grid

represented by Δt. The present and previous time-steps are represented by superscript 1 and 0 respectively.

EXPLICIT VS. IMPLICIT

The f term in Eq. 8 represents a weighting factor for the evaluation of properties with time, and can have any value from 0 to 1. When f is 0, all of the a^1 terms in equation 8 drop out, and only the a^0 terms remain. This indicates that all properties are evaluated at the previous time step, making the solution fully explicit. Inversely, when f is 1, all properties are evaluated at the present time-step, making the problem fully implicit. Any value of f between 1 and 0 makes the solution only partially implicit. After exploration of different weighting factors, we decided to use the fully implicit method.

CODING

Due to the 1D nature of the problem, the set of linear equations becomes tri-banded, and can be easily handled by a routine that takes advantage of the sparse nature of the matrix. One such routine, TDMA(Tri-Diagonal Matrix Algorithm)[4], was used in our analysis. The code was optimized to split up the calculation of properties between phase change and non-phase change regions. This cut down on calculation time, and allowed for a very fine mesh.

HOMOGENEOUS PLANE WALL WITH CONSTANT-TEMPERATURE BOUNDARY

The homogeneous plane wall with constant-temperature boundary was chosen for validation of our numerical method because of its simplicity and because of the existence of a closed-form analytical solution, which is given in non-dimensional form by[5]:

$$u(x,\theta) = \frac{4}{\pi}\sum_{l=0}^{\infty}\frac{\sin\left[(2l+1)\pi x\right]}{2l+1}e^{-(2l+1)^2\pi^2\theta}, \qquad \text{Eq 13}$$

where

$$u = \frac{T - T_o}{T_i - T_o}, \qquad \text{Eq 14}$$

$$x = \frac{X}{L}, \qquad \text{Eq 15}$$

and

$$\theta = \frac{\alpha t}{L^2} \qquad \text{Eq 16}$$

The discretization of the unsteady one-dimensional heat-conduction equation for this case was as described by Eq. 8 for all inner grid-points, with a boundary equation of $T_P = T_{in}$. The finite-difference solution with Δt=5e-4 sec, and Δx=1.25e-3 is plotted with the 100-term analytical solution in Figure 2. Also plotted in Figure 3 is the error fraction between the two solutions. These results gave us confidence in the discretization and grid size.

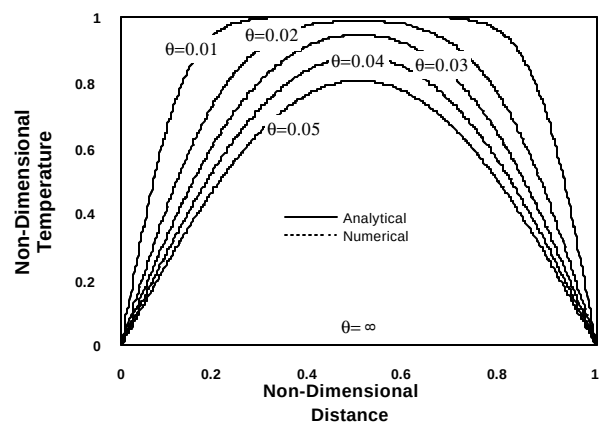

Figure 2 Validation of Constant Temperature Finite Difference Solution

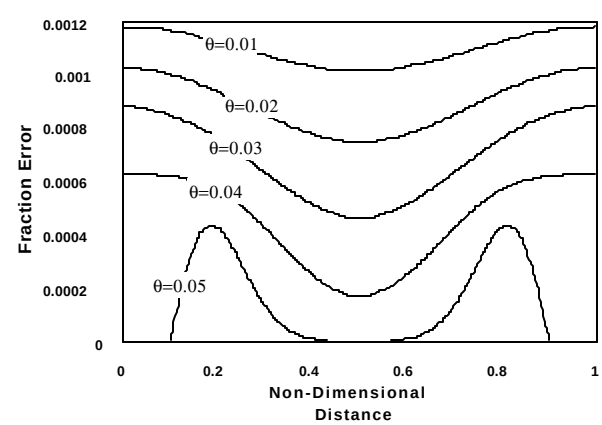

Figure 3 Constant Temperature Error

HOMOGENEOUS PLANE WALL WITH CONSTANT HEAT FLUX

The homogeneous plane wall with constant heat flux was essentially the same as the constant temperature problem, however with different boundary equations. As described by Patankar[4], the new boundary equation for the outside wall becomes:

$$a_B T_B = a_I T_I + b, \qquad \text{Eq 17}$$

where,

$$a_I = \frac{k_i}{(\Delta x)_i}, \qquad \text{Eq 18}$$

$$b = q_B, \qquad \text{Eq 19}$$

$$a_B = a_I. \qquad \text{Eq 20}$$

The inside wall is assumed to be adiabatic.

Once again, a closed form analytical solution[5] exists for this problem, and is plotted with the finite difference solution in Figure 4. The grid size and number of terms in the analytical solution are the same as those used in the previous simulation.

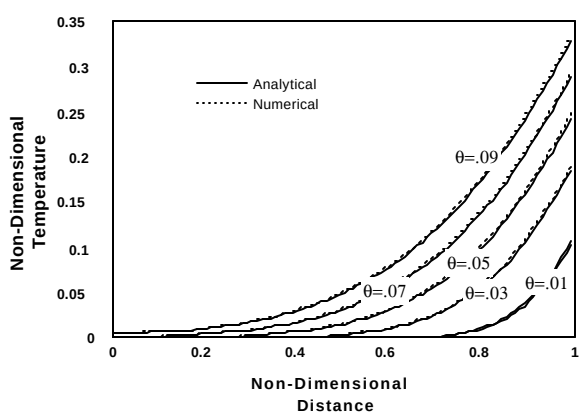

Figure 5 Validation of Constant Heat Flux Finite Difference Solution

COMPOSITE PLANE WALL WITH KNOWN HEAT FLUX AT BOUNDARIES

Using the experimental setup described earlier, a test was done using a plate coated with paint that contained no phase change material. This test was used to validate our numerical solution of a composite plane wall with know heat fluxes.

The case of a plane wall composed of two different materials required another modification of our discretization. As seen in Figure 1, the boundary between the two materials is assumed to lie on the interface between two control volumes. The thermal conductivity at the interface is taken to be the harmonic mean between the two materials. Eq. 9 then becomes:

$$a_E = \frac{2k_p k_E}{\Delta x(k_p + k_E)} \qquad \text{Eq 21}$$

Using the measured heat fluxes and a grid similar to those used in the previous simulations, the temperature was predicted, and graphed along with the measured data in Figure 5. For this, and the remaining simulations discussed, Δt=1.3e-3 sec, and Δx=1.3e-5m. This gave a Fourier number of 1.74, which proved to be plenty of resolution. It can be seen that the predicted temperatures overestimate the experimental data, but display the same profile. Due to good agreement of our numerical methods with exact solutions for similar cases, we conclude that the error was in the measurement of one, or more of the thermo-physical properties of the materials used.

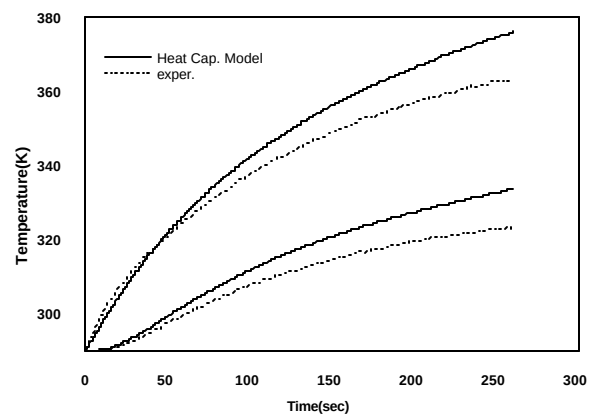

Figure 4 Experimental and Numerical Data for Composite Plate with no PCM

PHASE CHANGE MODEL

The phase change model was incorporated into the finite difference method used in the earlier studies, and used to simulate the temperature profile of three different experiments. In the first two experiments, the polyurethane coating was composed of 40% phase change mate-

rial. The results, shown in Figures 6 and 7 were encouraging in that the temperature profiles matched qualitatively well with the measured data. In both cases a valley, corresponding with the phase change period, occurs at nearly the same time. The temperatures are off by as much as 10 degrees K in some regions. The polyurethane coating in the third experiment contained 20% PCM. The numerical solution is plotted in Figure 8 along with the experimental data. Once again, an apparent bias between the experimental and numerical data is obvious. The profile once again matches qualitatively, but has a large amount of error.

The sources of error would appear to stem, once again, from improper values for the thermo-physical properties being studied. The constant over prediction of the solutions in Figures 8 and 9 could be due to a bias in the temperature or heat flux measurements, while the narrower temperature gradients between the surfaces as seen in Figures 6 and 7 might be attributed to a high value for thermal conductivity. Indeed, if we lower the thermal conductivity of both materials by 30% in our numerical solution, the results show a nearly perfect match between predicted and measured data, as shown in figure 10.

CONCLUSIONS

We have developed and tested a model for predicting the heat transfer through a composite which contains a phase change material. A finite difference numerical method was implemented to test the model against experimental results. The model appears to give a good qualitative description of the process, but is consistently shifted from the experimental data. More confidence should obtained in the data with future experiments.

BIBLIOGRAPHY

1. Maguire, M, M. Gambill, J. Menousek, "Microencapsulated Phase Change Material, Vol. 1. Aircraft Applications," WR-TR-96-3142, Flight Dynamics Directorate, Wright Laboratory, WPAFB, OH, January 1996.

2. Bowman, W. J. and D. A. Brown, " Heat Capacity Model for a Mixture Containing a Phase Change Material," AIAA Paper # 98-2764, 7th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, June 15-18, 1998.

3. Yao, L. S., J. Prusa, "Melting and Freezing," Advances in Heat Transfer, Vol 19, pp 1-95, 1989.

4. Patankar, S. V. "Numerical Heat Transfer and Fluid Flow"

5. Carslaw, H. S., and J. C. Jaeger, Conduction of Heat in Solids, 2nd Edition, Oxford, 1971, p 242.

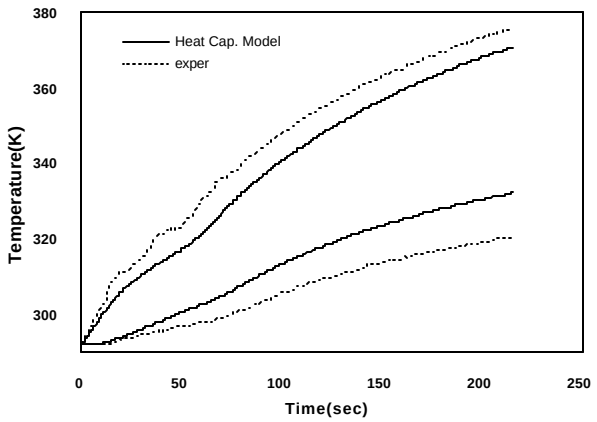

Figure 7 Results of First 40% PCM Experiment

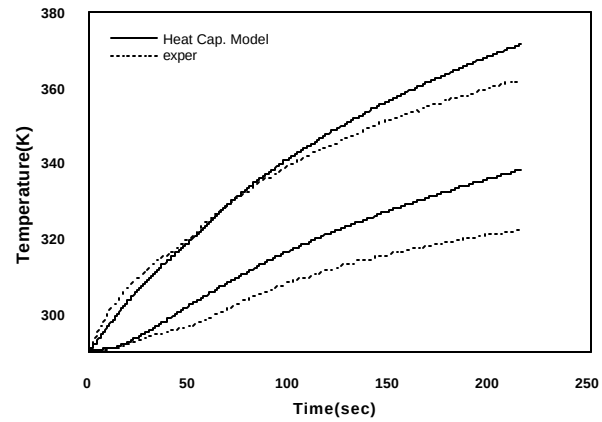

Figure 6 Results of 20% PCM Experiment

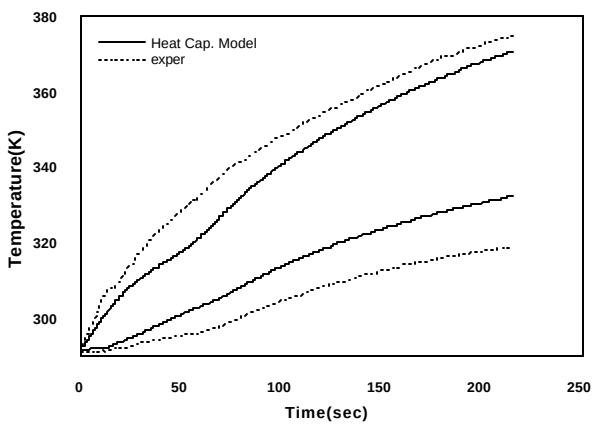

Figure 8 Results of Second 40% PCM Experiment

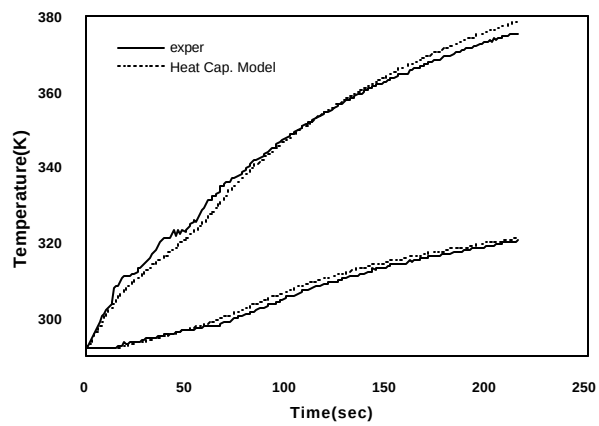

Figure 9 40% TMD Simulation with 30% reductions in k

Table 1- Measured Material Properties

	Composite	Coating, 0% pcm	Coating, 25% pcm	Coating, 40% pcm
K (W/m-K)	0.38	0.29	0.29	0.29
c (J/kg-K)	1050	960	1250	1420
ρ (kg/m^3)	1440	1250	1150	1090
Thickness (mm)	3.0	Variable	Variable	Variable