Mass conservation in modeling moisture diffusion in multi-layer carbon composite structures

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Abstract

Moisture diffusion in multi-layer carbon composite structures is difficult to model using finite difference methods due to the discontinuity in concentrations between adjacent layers of differing materials. Applying a mass conserving approach at these boundaries proved to be effective at accurately predicting moisture uptake for a sample exposed to a fixed temperature and relative humidity. Details of the model developed are presented and compared with actual moisture uptake data gathered over 130 days from a graphite epoxy composite sandwich coupon with a Rohacell® foam core.

Key words: Finite difference modeling, Moisture diffusion, Rohacell®, Gaphite epoxy composites

1. Introduction

Rockets, such as the Delta and Atlas, are exposed to a varied environment, including high levels of humidity and moisture, which can adversely affect various components and structures. Of particular interest are rocket fairings, often fabricated from graphite epoxy composite (GEC). These have been shown to absorb significant amounts of water while in a high humidity environment leading to structural weakening during ascent heating[1]. Consequently, methods for determining the water content of GEC structures are of interest, and one such method is by computation using a diffusion model. This approach assumes the GEC is dry at fabrication, requires continuous monitoring of the GEC temperature and humidity environment, and needs well established material parameters, but is inexpensive and non-intrusive.

This paper discusses a one dimensional finite difference based diffusion model for a three layer composite structure composed of a GEC-foam-GEC sandwich arrangement, similar to that seen in some rocket fairings. Others[3] have created similar models, but lack a thorough explanation of the boundary conditions needed to enforce water mass conservation and have not compared their models against long term experimental data. In the present discussion we explain in detail how mass conservation over the GEC-foam interface is treated and then compare the resultant model against the moisture uptake seen by a GEC-foam-GEC sandwich sample over a 130 day period.

2. Three Layer Diffusion Model

The fairing material physically consists of five layers, formed by bonding a GEC face sheet to each side of a Rohacell® foam core using a thin adhesive. Due to their thin size with respect to the GEC and foam, the glue layers were neglected for modeling the overall diffusion behavior. However, the three layer model created can easily be extended to include the thin adhesive layer.

The model consists of two main computational techniques that will be discussed below. The first uses a standard finite difference equation based on Fick's law to compute the water concentration for the next step in time. This technique cannot be used at the boundary between dissimilar materials because the moisture concentration is discontinuous across the interface. Therefore, a second mass conserving technique was created to compute the moisture concentration across that boundary.

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2.1. Discrete representation of Fick's law

Fick's law of diffusion in differential form is

$$\frac{\partial c}{\partial t} = \vec{\nabla} \cdot (D\vec{\nabla}c), \tag{1}$$

where D is the diffusivity and c is the water concentration [2]. After integrating this equation over a volume and applying the Divergence Theorem, the resulting form tells us that the change in water in that volume is the net difference between what goes in and out of the surface that bounds the volume. The present problem can be reduced to a simple one dimensional equation by assuming the diffusivity and concentration only vary across the thickness of the sample. Integrating Equation 1 over a cuboid shaped volume with each face perpendicular to a coordinate axis and assuming that the concentration varies only along the x-axis yields the following equation:

$$A \int_0^h \frac{\partial c}{\partial t} dx = A(D\frac{\partial c}{\partial x} |_1 - D\frac{\partial c}{\partial x} |_2), \tag{2}$$

where A is the area of each of the cuboid faces normal to the x-axis, numbered 1 and 2 above, and h is the distance between the two faces.

For sufficiently small time and spacial intervals, the following discrete form can be used to perform numeric computations:

$$\frac{1}{\tau}(c_i^{n+1} - c_i^n) = \frac{1}{h^2}(D_{i-1}c_{i-1}^n - 2D_ic_i^n + D_{i+1}c_{i+1}^n), \tag{3}$$

where τ is the time interval between adjacent time steps, n and $n+1$, and h is the spacial interval between adjacent spacial nodes, i and $i+1$. This equation was used to find the time evolution of the concentration c_i^{n+1} at each point on the grid except at the boundary layers. This method is often referred to as the forward in time and centered in space (FTCS) approach and is stable if $2D\tau/h^2 < 1$ [4].

2.2. Boundary conditions and conservation of mass

The FTCS method works well until a discontinuity in moisture concentration is encountered at the border between two dissimilar materials. Springer [5] approaches this in the "W8GAIN" Fortran code by applying two boundary conditions at the interface between the two layers.

The first is a reasonable statement that the relative humidity, ϕ, is equal across the boundary. This can be used to join together the empirical relationships between relative humidity and concentration for each of the materials, $c1_k^{i+1} = \rho_1 a_1 \phi_1^b$ and $c2_1^{i+1} = \rho_2 a_2 \phi_2^b$, where $c1$ and $c2$ are the moisture concentrations on either side of the boundary in materials 1 and 2, shown in Figure 1. ρ_1 and ρ_2 are the dry densities of each of the materials and a_1, b_1, a_2, b_2 are the empirical coefficients of materials 1 and 2, respectively. Equating ϕ on each side of the boundary yields:

$$c2_1^{i+1} = \rho_2 a_2 (c1_k^{i+1}/\rho_1 a_1)^{b_2/b_1}. \tag{4}$$

However, the second condition mentioned by Springer,

$$D_1\frac{\partial c1}{\partial x} = D_2\frac{\partial c2}{\partial x}, \tag{5}$$

is not reasonable. This condition states that any moisture that flows in from one face of a small cuboid volume leaves the opposing face with no accumulation, which is not physical since no water remains to accumulate at the boundary. Therefore, another boundary condition is needed and can be found by enforcing conservation of mass in the finite volume surrounding the border between layers (refer to Figure 1).

Let c_b be the accumulated moisture concentration at the boundary, determined by what flows into the left hand side of finite volume in material 1 and what flows out of it's right hand side in material 2. This is represented mathematically by Equation 6 below:

$$c_b^{i+1} = c_b^i + \frac{\tau}{h}(D_1\frac{c1_{k-1}^i - c1_k^i}{\frac{3}{4}h} - D_2\frac{c2_1^i - c2_2^i}{\frac{3}{4}h}), \tag{6}$$

where material 1 has been divided into k cells. The nodes for $c1_k$ and $c2_1$ are $\frac{1}{4}h$ away from c_b and $\frac{3}{4}h$ away from $c1_{k-1}^i$ and $c2_1^i$, respectively.

From Figure 1, its easy to see that in order to conserve mass,

$$Ahc_b^{i+1} = \frac{Ah}{2}c1_k^{i+1} + \frac{Ah}{2}c2_1^{i+1}. \tag{7}$$

Simplifying and rearranging terms yields,

$$c1_k^{i+1} = 2c_b^{i+1} - c2_1^{i+1}. \tag{8}$$

Now Equations 4 and 8 provide enough information to progress across the boundary. Substitution of Equation 4 into Equation 8 gives us an equation for c_b^{i+1} as a function of $c1_k^{i+1}$:

$$c_b^{i+1} = 1/2(c1_k^{i+1} + \rho_2 a_2 (c1_k^{i+1}/\rho_1 a_1)^{b_2/b_1}). \tag{9}$$

The value of c_b^{i+1} is determined from Equation 6, leaving only $c1_k^{i+1}$ as unknown. Unfortunately, due to its non-linearity, this equation is difficult to invert. Some [6] assume the concentration is linearly related to the relative humidity, but this leads to error when $b_1 \neq b_2$. However,
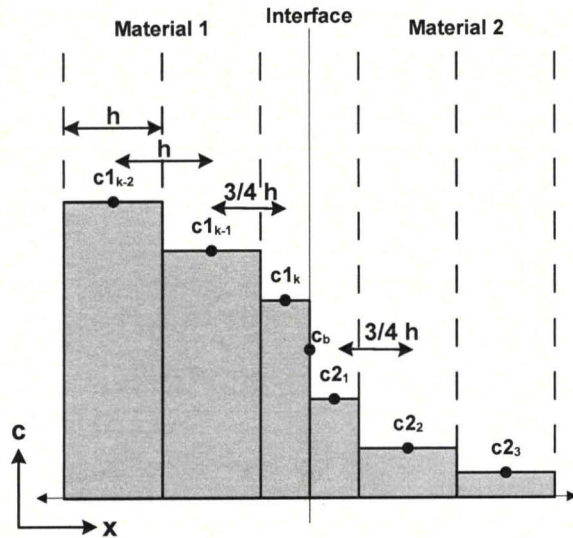
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Figure 1: Finite volumes of width h are shown near the boundary between materials 1 and 2. The volume around node c_b is made up of two different materials, one with concentration $c1_k$ and the other $c2_1$.

by allowing $c1_k^{i+1}$ to vary between 0 and $\rho_1 a_1$ in fine increments, a polynomial fit can be applied to the data to get $c1_k^{i+1}$ as a function of c_b^{i+1}. A tenth order fit was performed for this work, but lower orders may be used depending on desired accuracy and the degree to which the empirical values for b vary from 1. Once $c1_k^{i+1}$ is calculated, $c2_1^{i+1}$ is easily found from Equation 8.

Equation 3 works well for the remaining nodes outside the boundary. However, it must be modified slightly when calculating $c1_{k-1}$ and $c2_2$ to account for the change in node spacing near the boundary (3/4 h vs. h). Once each of concentrations for the next time step are computed, the final step is to sum up the water mass in each finite volume for a given time. This is then used to construct the plot of the total water mass vs. time. As a self consistency test, the moisture rate flowing in through the outer faces was integrated with respect to time and proved to be identical to the total achieved by summing up the moisture distribution through the sample at each step in time.

3. Experimental Data

A graphite epoxy composite sandwich with Rohacell foam core was analyzed to determine its moisture uptake properties. Moisture uptake measurements were made on a sample of the foam core and a complete sandwich coupon. The manufacturer, United Launch Alliance (ULA), provided the key information on the graphite epoxy face sheet. The samples were vacuum

dried and then subjected to 37.8°C and 85.0% RH in an environmental chamber. Periodic weight measurements were made during the wetting process to determine change in mass over time.

3.1. Foam Core Results

Two samples (Figure 2) of 110 WF Rohacell were tested, which according to the manufacturer has an average density of 0.110 g/cm^3 over a large sheet. The measured densities of the samples tested are 0.11 g/cm^3 and 0.13 g/cm^3, showing some construction variation. The mathematical expression for the normalized moisture uptake is given by Springer [5] as

$$\frac{M(t) - M_i}{M_m - M_i} = 1 - \frac{8}{\pi^2} \sum_{j=0}^{\infty} \frac{1}{(2j+1)^2} e^{-(2j+1)^2 \pi^2 Dt/h^2}, (10)$$

where, $M(t)$ is the measured mass as a function of elapsed time, t, M_i is the initial mass, M_m is the maximum mass, h is the thickness of the sample, and D is the diffusivity. Mathematica® [8] was used to find the diffusivity by restricting the summation to the first 100 terms and applying the Fit function to the data sets. The resulting plots are shown below

Figure 2: Two samples of 110 WF Rohacell Foam were vacuum dried and subjected to moisture uptake testing in an environmental chamber.

Equation 10 applies to an infinite sheet of fixed thickness. Since the sample's length and width aren't sufficiently large when compared to the thickness, a correction needs to be applied to take out the effect of the increased uptake due to the open sides. This corrected diffusivity, D_c is provided in terms of the length, width, and thickness (l, w, and h) by Springer as:
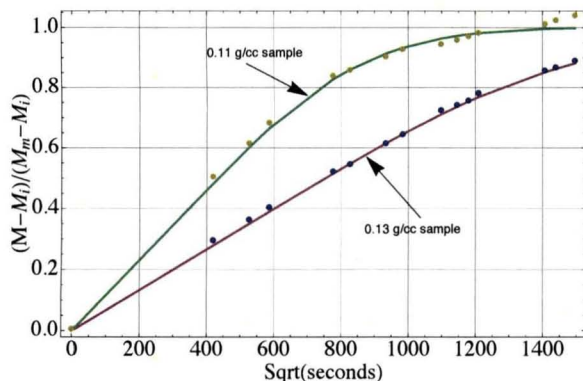
$$D_c = D/(1 + \frac{h}{l} + \frac{h}{w})^2. \quad (11)$$

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Figure 3: Normalized moisture uptake data and fitted curves for each of the Rohacell foam samples. The fitted diffusivities are 4.2 x 10^{-7} cm^2/sec for the 0.11 g/cm^3 sample and 3.2 x 10^{-7} cm^2/sec for the 0.13 g/cm^3 sample.

The corrected values of diffusivity for our samples are 2.8 x 10^{-7} cm^2/sec for the 0.11 g/cm^3 sample and 2.0 x 10^{-7} cm^2/sec for the 0.13 g/cm^3 sample.

3.2. GEC-Foam-GEC Sample Results

Epoxy and aluminum tape were applied to the edge of a GEC-foam-GEC sample coupon to minimize moisture uptake directly into the foam core. The sample was dried in a vacuum chamber for several weeks and then placed in the environmental chamber on a precision scale for approximately 130 days at constant temperature and humidity (37.8°C and 85.0% RH). The mass was collected from the scale at regular intervals and stored along with a time-stamp on a laptop computer.

With the exception of the diffusivity of the Rohacell, the diffusion properties of the sample's materials have been previously determined. ULA provided the needed values for input to our model program, which are summarized in Figure 4 below.

	Density (g/cc)	a	b	D (cm^2/sec)	Area (cm^2)	h (thickness) (cm)
facesheet	1.61	1.5	1.7	2.00E-09	248	0.142
core	0.111	11	1.9	2.80E-07	248	1.27

Figure 4: This contains a summary of the sandwich material parameters.

The data from the moisture uptake test is plotted along with the predicted output in Figure 5. The unusual data behavior after the 100 day mark is believed to be due problems with the scale, which failed entirely after about 130 days.
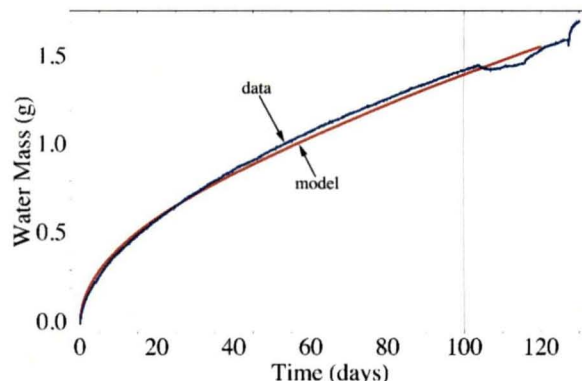

Figure 5: This plot shows the moisture uptake of a fairing coupon in an environmental chamber at 37.8°C and 85.0% RH for about 130 days. Since the scale was also exposed to this environment, the anomalous data after the 100th day may be related to possible condensation within the scale electronics, which experienced a hard failure around the 130th day. The 2nd plot shows the output predicted by our diffusion model using the diffusion parameters for the facesheet and foam core.

4. Conclusion

The finite difference method coupled with a mass conserving approach at the boundaries proved to be effective at predicting moisture uptake for fixed RH and temperature. The output of the multi-layer diffusion model is in close agreement with data collected on the moisture uptake of a GEC-foam-GEC sample coupon. Future work will focus on incorporating variations in temperature and relative humidity into the model to better represent the environment seen by fairing material between fabrication and liftoff.

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