3D Thermal-Diffusion Analysis on a Moisture Loaded Epoxy Sample

S. Madduri*[1], W. Infantolino[2], and B.G.Sammakia[1]
[1]Department of Mechanical Engineering
[2]Integrated Electronics Engineering Center (IEEC)
* IEEC, P.O. Box 6000, Binghamton, NY 13902-6000
smaddur1@binghamton.edu

Abstract: Hygroscopic swelling due to moisture absorption is an important concern in electronic packages that are exposed to humid environments. This results in hygroscopic strains that may lead to package failure.

COMSOL's multiphysics module was used to simulate an experiment in which the hygroscopic swelling in an epoxy material was measured throughout a temperature ramp. A simultaneous solution was sought for the temperature and moisture concentration distribution in a moisture loaded epoxy sample.

Initially the multiphysics problem was broken down into two separate cases - transient heat transfer analysis and transient diffusion analysis. The diffusion analysis required use of a stepped boundary condition on the surface of the part. Results from the transient heat transfer analysis were in good agreement with the experimental solution. However, a physically unrealistic result (local concentrations above initial value with drying of the epoxy material) was found in the solution for the transient diffusion analysis.

Several options that aid convergence were run on the model in an attempt to resolve the problem. Results from the individual cases as well as from the multiphysics model with both the cases considered together are presented in this paper.

Keywords: multiphysics, transient diffusion analysis, transient heat transfer analysis

1. Introduction

A wide variety of epoxy materials are used in electronic packaging. These epoxy materials are hydrophilic in nature and absorb moisture when exposed to humid environments. Hygroscopic swelling is the expansion of a material due to moisture absorption [1]. Swelling can induce stresses in the package that can lead to failure.

A Digital Image Correlation (DIC) technique was used to measure the moisture swelling in the epoxy material. A moisture loaded epoxy sample was subjected to a temperature ramp in a convection heat oven. Due to the temperature ramp, moisture loss occurs in the sample and this leads to a change in concentration distribution in the material. The distribution of moisture concentration in the epoxy sample throughout the DIC scan was estimated using a numerical model [2]. The ramp was conducted in a temperature range below the glass transition temperature of the test material.

As an extension to the work done in [2], a multiphysics model was proposed to obtain a simultaneous solution for the temperature, and moisture concentration distribution in the epoxy sample. A moisture stress analysis would also be included in this simulation to determine the effect of non-uniformity in moisture concentration for elevated temperature measurements.

COMSOL multiphysics was used to simulate the DIC experiment in an attempt to solve the temperature and moisture concentration simultaneously.

2. Problem Definition

The multiphysics problem was initially divided into two separate cases – a transient heat transfer analysis and a transient diffusion analysis.

2.1 Transient Heat Transfer Analysis

Assuming a uniform heat transfer coefficient on all surfaces of the epoxy sample, the oven temperature was applied to the sample to obtain the sample temperature profile. This was compared with the actual sample temperature measured from the experiment.

The results show good agreement between both temperature profiles. Figure 1 shows the sample temperatures from the experiment and numerical analysis.

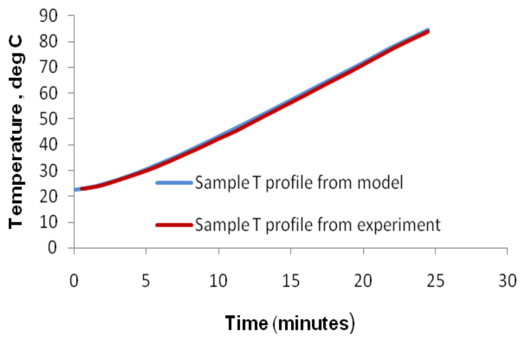

Figure 1. Comparison of sample temperature profiles from numerical analysis and experiment

2.2 Transient Diffusion Analysis

Moisture loss during the experimental measurement leads to a degree of non-uniformity in the moisture concentration in the sample. The distribution of moisture concentration in the sample throughout the DIC scan was estimated numerically using a transient diffusion analysis in COMSOL multiphysics.

2.2.1 Diffusivity measurements

Moisture transport by diffusion is modeled by Fick's law. For a one-dimensional diffusion problem, this is expressed as (1):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial^2 z} \quad (1)$$

Where D is the diffusion coefficient (mm^2/s); C is the local moisture concentration (g/mm^3); and t is the time (seconds).

The diffusion coefficient was determined using moisture desorption data for the epoxy material using a non-linear regression method [3]. The reason for using desorption instead of absorption data was to be consistent with the DIC scan which is a desorption process. A sample saturated with moisture at 85°C and 85 % RH was used for desorption scans at different temperatures. The desorption temperatures chosen were 85°C, 75°C, 65°C, 55°C, and 35°C. Periodic weight loss measurements were recorded throughout the desorption scan. Figure 2 shows the weight loss data recorded for different temperatures. This data was the basis for the diffusivity calculations.

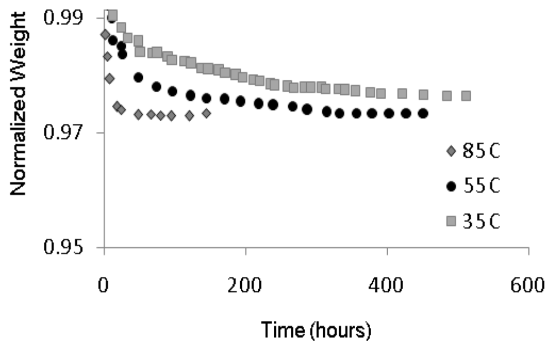

Figure 2. Weight loss data as a function of time

Figure 3 shows the diffusivity as a function of temperature from the regression method for the epoxy material tested.

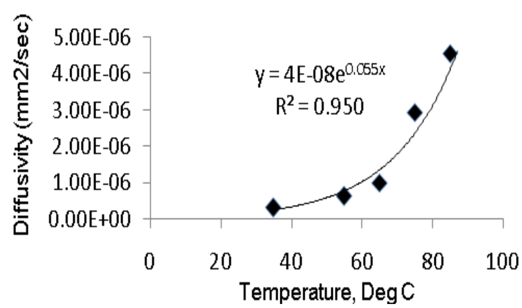

Figure 3. Diffusivity as a function of temperature

The diffusivities at different times along the DIC scan were computed using the sample time / temperature profile and the curve fit from the calculated diffusivity values (shown in Figure 3). These were applied in the model of the transient diffusion analysis. The sample was initially set to the percent saturated moisture content (3.2033) of the material measured at the beginning of the DIC scan. The diffusivity based on the sample temperature profile from the experimental DIC run was simulated in the model and the moisture distribution in the sample was determined as a function of time.

Figure 4 shows the moisture distribution in the sample at the end of the first time interval in the DIC ramp (time= 30 seconds) obtained from the numerical model. A one-eighth section of the sample was modeled based on symmetry. The results indicate a small region of non-uniformity in moisture concentration at the surface of the test material in the temperature range tested.

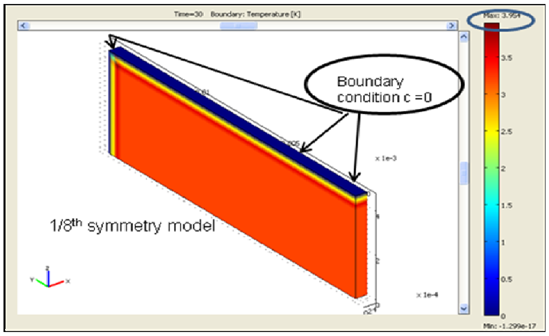

Figure 4. Moisture distribution in the epoxy sample

When the nodal concentration was plotted, results indicated a physically unrealistic result (a concentration value, 3.954, which was greater than the initial concentration of 3.2033). This was located near the sharp gradient region at the surface. This is probably due to the presence of the spatial discontinuity near the surface of the part (zero concentration on the surface).

The nodal concentration from this analysis was compared to the nodal concentration obtained from the exact same simulation (same geometry, material properties, mesh sizes and solution time step sizes) that was run using different software [2]. Results from that simulation indicate a maximum concentration value in the nodal solution equal to the initial condition.

Results from both the simulations were compared at different times (short and long times) and nodal concentrations in different locations in the model were compared. Using the solution from the other software as a reference (software that did not have the physically unrealistic peak concentration value above the initial maximum value), a percent relative error value was computed between the concentration values from both the solutions. These are presented in Table 1.

Table 1. Percent relative error in concentration values at different times and different regions across the sample

Time (minutes)	**Percent Concentration Difference (Thicker Cross Section- DIC Sample)**		
	Center of Sample	**Location where Maximum occurred in COMSOL**	**Within Sharp Gradient Region**
0.5	0	23	0
133	0	7.26	0
233	0	6.42	0.12
500	0.62	0.71	2.31
583	1.91	0	3.94
666	3.11	1.24	5.63

Both the solutions were compared for a simulation run on a thinner cross section sample (thought to be more representative of the thickness in an actual package application). The results from this analysis are presented in Table 2.

Table 2. Percent relative error value in concentration values at different times and different regions across the sample

Time (minutes)	**Percent Concentration Difference (Thinner Cross Section)**		
	Center of Sample	**Location where Maximum occurred in COMSOL**	**Within Sharp Gradient Region**
0.5	0.49	24	0.52
47	14.39	0	10.36

Results indicate that the mathematical problem that created the unrealistically high concentration was not resolved at longer times. Figures 5 and 6 show the corresponding plots.

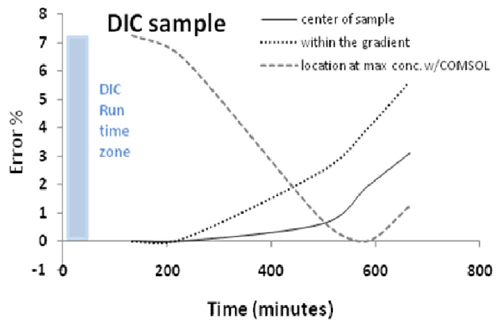

Figure 5. Percent error in concentration value across the sample (thicker cross section)

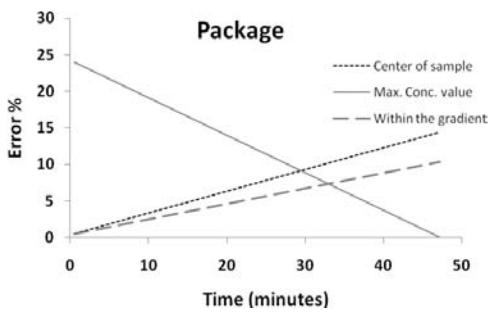

Figure 6. Percent error in concentration value across the sample (thinner cross section)

3. Numerical study on solution convergence

3.1 Transient heat transfer analysis

Based on the above results, further analysis was done to study the mathematical problem found in the solution. A simple transient heat transfer analysis with a spatial discontinuity at the surface was done. A copper block was considered for the analysis. It was assumed that the high thermal conductivity of copper will reduce the steepness of the gradient occurring at the boundary unlike the current epoxy with a very low diffusivity. The material properties were picked from the COMSOL material library. The block was initially set to a temperature of 100^{o}C and the boundary was set to a temperature of 0^{o}C. A 1/8th symmetry model was analyzed.

Results indicated the mathematical problem in solution at the initial time interval (0.1 to 10 sec) and it faded out with longer times (15 to 30 sec). Though the longer time solution showed no peak, the earlier history does affect the solution at later times. A difference in the solution was found with the other software. Figure 7 shows the temperature distribution in the copper block. Nodal temperatures along the central diagonal passing through the volume of the sample are shown in Figures 8 and 9.

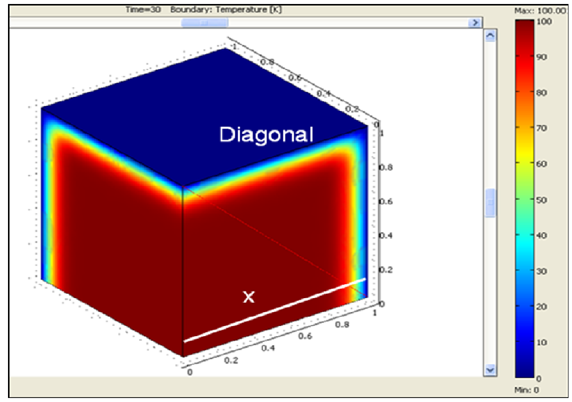

Figure 7. Temperature distribution in the Cu block

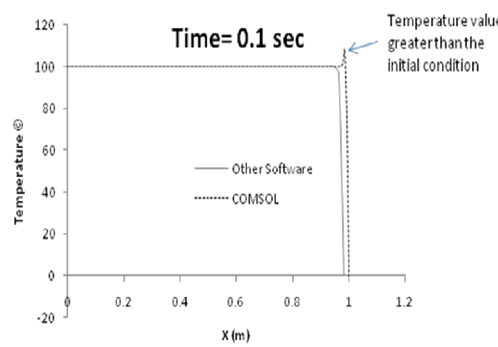

Figure 8. Nodal temperatures along central diagonal at time interval of 0.1 second

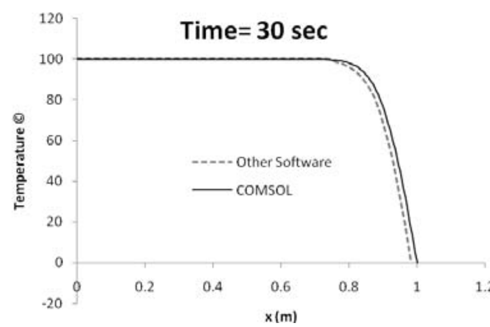

Figure 9. Nodal temperatures along central diagonal at the end of run (30 seconds)

Based on the observation from the previous analysis, the current test model was run for longer times. The model was initially run for the total experiment time of 24 min. The problem showed up in the solution for this time frame; however it improved at very long time intervals (approximately 500 min). A concentration above the initial value may not be observed at very long times, however, because of the previous history of the error in the solution at short times, the longer time values are still in error. These longer times may be more representative of the actual application (package) time.

Strain values were estimated for the solution at short and long times and compared with the solution obtained from the other software. This was done to compare the solution across the total sample volume, rather than a local point wise peak value. The estimated strain values along with the difference in solution in terms of a percent error are given in Table 3.

Results indicate that the strain values for both the solutions are in better agreement at the longer time intervals. Run times for a given reduction in error are model dependent.

Table 3. Percent error in strain values

	Strain (%)	
	Time (30 seconds)	**Time (30,000 seconds)**
Thicker cross section (DIC test sample)	11.94	3.84
Thinner cross section	13.11	7.69

3.2 Further analysis

Several options that aid convergence were run on the model in an attempt to resolve the problem. These included mesh refinement, time stepping options, using different solvers, and using a different element type. These did not help resolve the problem.

Potential solutions from COMSOL technical support and review of prior literature included using a ramp boundary condition and an unstructured mesh. These are presented in the next section.

3.2.2 Ramp boundary condition

The technical support at COMSOL suggested using a ramp boundary condition in space. However, the concentration gradient is the solution we seek from the analysis and hence it cannot be defined as an input. Therefore, a ramp boundary condition in time of the surface boundary condition was used instead. The objective was to determine if a short ramp could be used that would prevent the mathematical problem and not have a significant effect on the solution at the time of interest.

Figures 10 and 11 present nodal concentrations from the COMSOL solution with two different ramp boundary conditions. Results indicated a larger peak in the solution at the sharp gradient region compared to the stepped boundary condition even with longer times.

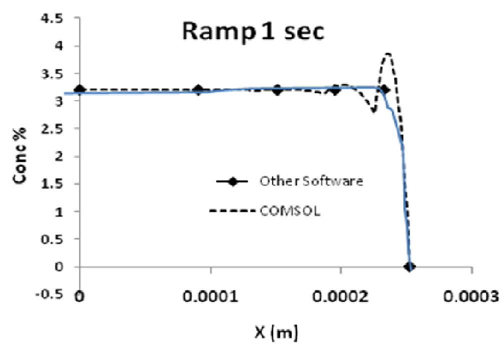

Figure 10. Nodal concentration plot for a short ramp (1 second)

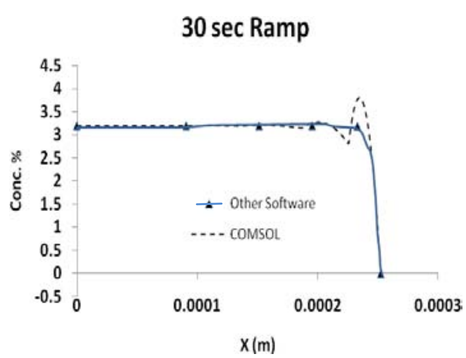

Figure 11. Nodal concentration plot for a longer ramp (30 second)

3.3 Unstructured mesh

Several runs were made using an unstructured mesh, with varying degrees of refinement (previous runs done with mapped mesh). The mathematical problem seemed to improve somewhat (a relative reduction in the peak point concentration value) compared to the mapped mesh case, but the problem was still present. It was concluded that this option was not viable for preventing the mathematical problem.

Figure 12 shows a concentration plot from one of the unstructured mesh cases. The mathematical problem (in the form of noise) near the sharp gradient region is clearly shown on the nodal concentration plot in Figure 13.

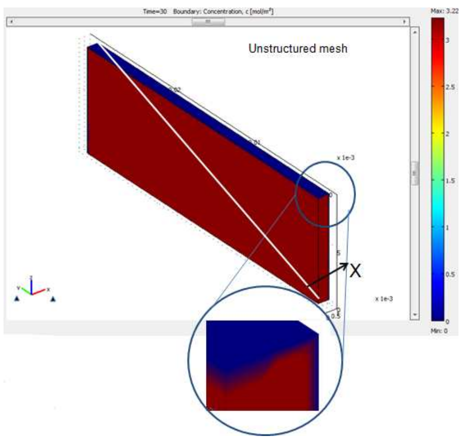

Figure 12. Concentration distribution in epoxy material

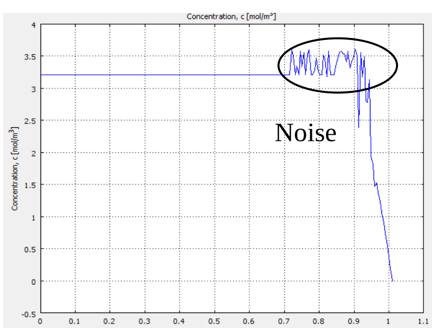

Figure 13. Nodal concentration plot

4. Multiphysics problem

A thermal-diffusion analysis with a simultaneous solution for temperature and moisture concentration in the material was run using the multiphysics module.

Figure 14 shows the temperature and moisture concentration distributions along with the corresponding nodal results plotted.

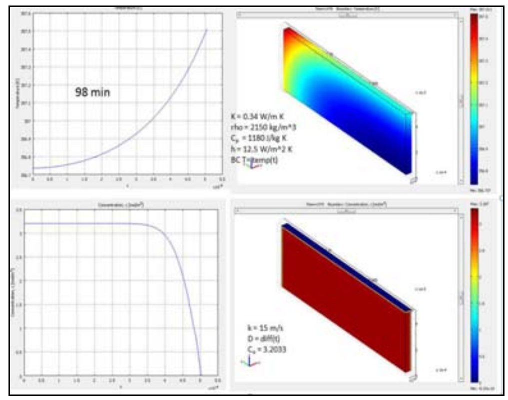

Figure 14. Multiphysics problem solution considering the thermal-diffusion analysis together

Results for the temperature distribution were similar to those found in the transient heat transfer analysis. No mathematical problem was found in that portion of the solution. However, results from the transient diffusion analysis indicated the mathematical problem in the nodal concentration plot similar to the one found in the transient diffusion analysis considered alone. The maximum concentration value is greater than the initial condition (shown in Figure 15)

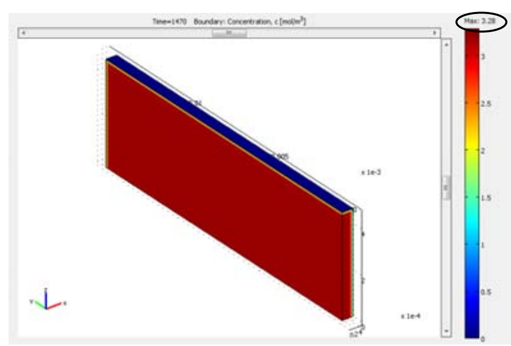

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Figure 15. Concentration distribution in sample showing a max. concentration value of 3.428 which is greater than the initial condition of 3.2033

Figure 16 shows the concentration plots with time along the central diagonal across the volume of the sample. The mathematical problem (peak) smoothed out with time along a particular nodal set. However, the maximum concentration value was still greater than the initial condition across the total volume of the sample. This indicates that the local concentrations at longer time intervals are likely to not be reliable.

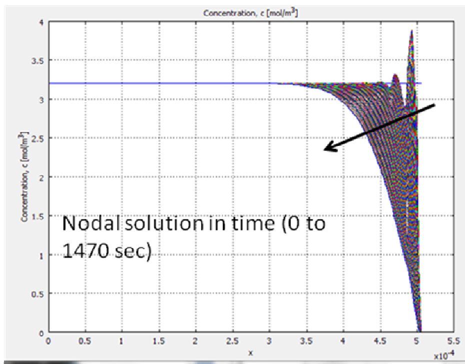

Figure 16. Nodal concentration plots with time along the central diagonal passing through the volume of the sample

5. Summary and conclusions

The COMSOL solution was in excellent agreement with the experimental solution for the transient heat transfer analysis. However, results indicated a physically unrealistic result in the transient diffusion analysis. Several options that aid convergence were run on the model in an attempt to resolve the problem. These options did not prove viable in solving the problem.

A simple transient analysis was run with a material selected from COMSOL's database. Results showed the peak value above the initial value at shorter time intervals that eventually faded out with time. The local concentration value that was higher than the initial condition will eventually decrease below the initial condition due to diffusion, however, once the value gets below the initial value does not make it a correct or an error free solution. The earlier history of the error will still affect the solution at longer times.

All the simulations (except the multiphysics case) presented in this paper were run using another commercially available software. Results were in excellent agreement with the experimental results and the COMSOL solution for the transient heat transfer case. Results for the other cases were also compared. Solutions (strain values) were in better agreement over longer time intervals, for the transient diffusion case. However, the mathematical problem still existed in the COMSOL solution even for the longer times

It was concluded that COMSOL could not be used to simulate this problem in the short term and long term, due to the presence of a mathematical problem in solution. Though the magnitude of error (in terms of local strains measured) reduced for longer time intervals, the history of the unrealistic result affects the final solution. Results at longer times did not correlate well with results obtained from the other software.

6. References

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