Finite Element Modeling of Anomalous Moisture Diffusion with Dual Stage Model

Xuejun Fan and Vishal Nagaraj
Department of Mechanical Engineering
Lamar University
PO Box 10028, Beaumont, TX 77710, USA
Tel: 409-880-7792, E-mail: xuejun.fan@lamar.edu

Abstract

In this paper, finite element modeling of anomalous moisture diffusion using commercial finite element code is developed. The modeling method and numerical implementation is based on a dual stage model with both stages described by Fickian terms mathematically. The method is also extended to desorption process at reflow, in which the permanently trapped moisture content is a function of temperature. This paper details the finite element modeling implementation steps for both moisture absorption and desorption. The results are compared to the analytical solutions, and are also compared to the experimental data. A single script using ANSYS APDL is developed for the whole process including absorption and desorption phases.

1. Introduction

The moisture absorbed by a polymer occurs in two states, mobile and bound [1, 2]. In the mobile state, water molecules from the environment migrate to the microscopic pores, free volumes, or voids in the material to achieve concentration equilibrium. The process is similar to a typical mass concentration gradient driven diffusion process, and can be described well by Fick's laws. In the bound state, the water molecules bind with epoxy resins through hydrogen bonding. Two types of bound water are found in epoxy resins [3], as classified as Type I or Type II bonding, depending on the difference in the bond nature and activation energy. Type I bonding corresponds to a water molecule which forms a single hydrogen bond with the epoxy resin network. This water molecule possesses a lower activation energy and is easier to remove from the resin. Type II bonding is a result of a water molecule forming multiple hydrogen bonds with the resin network. This water molecule, therefore, possesses a higher activation energy and is correspondingly harder to remove. Higher temperature and longer exposure time is required to remove the Type II bond water molecules [3].

Moisture absorption exhibits both processes: mobile water and bound water in materials, and the later is referred to the non-Fickian diffusion process. The experimental results of moisture absorption for epoxy mold compounds (EMCs) at 85°C/85%RH, followed by desorption at the same temperature (85°C/0%RH) show that moisture absorption experiences two-stage diffusion, and the non-Fickian diffusion is nonreversible at the same temperature, at least for a period of 2 weeks. However, higher temperature from 100°C to 260°C allows more bound water removed, and experimental data also show reasonable fit following Fickian diffusion model in reflow process [4,5].

For finite element modeling of moisture diffusion in IC packages, Tay et al. [6] first used the normalized approach for the moisture diffusion analysis under absorption. Galloway et al. [7] introduced thermal-moisture analogy methodology to analyze moisture diffusion. Wong et al. [7] developed an alternative normalized variable called "wetness", which is defined as the ratio of the moisture concentration over the saturated moisture concentration. For moisture diffusion modeling in reflow process, Xie et al. [9,10] introduced the direct concentration approach (DCA). In the DCA, the moisture concentration is used directly as a basic field variable, which is discontinuous at interfaces. Continuity equations are applied at the interfaces using constraint equations.

In this paper, commercially available finite element software will be used for modeling non-Fickian diffusion process. A dual-stage diffusion model in terms of Fickian parameters for both stages, has been developed recently by one of the authors [4,11]. This paper will report the finite element implementations of this model with commercial finite element software.

2. Mathematical Models

The dual stage model applies the notion that Fickian and non-Fickian diffusion occur simultaneously throughout the process. The stages are distinguished by which behavior is most dominant. In the first stage, Fickian behavior is dominant. As the relaxation rate increases and diffusion rate slows, the non-Fickian behavior appears signaling the start of the second stage. If C_1 is the function of concentration due to Fickian behavior and C_2 represents the concentration due to non-Fickian behavior, superpositioning these two functions gives the total concentration of the sample, as follows,

$$C(x,t) = C_1(x,t) + C_2(x,t) \tag{1}$$

where C_1 represents the moisture concentration due to Fickian diffusion while C_2 is non-Fikican contribution to moisture concentration. Eventually the total saturation will be reached after the relaxation process is complete. The concept of dual stage model has been applied to several different diffusion processes, such as Carter and Kibler's Langmuir-Type Model [12] or Gurtin and Yatomi's "free" and "trapped" phase model [13]. Those models provide good agreement with experimental data, but introduce additional parameters and mathematical complexity. Alternatively, the second stage can be also modeled in Fickian terms for mathematical simplicity and comparability [4,11]. It should be noted that the second stage (C_2) is an irreversible, non-Fickian process. Equation (1) becomes

$$C(x,t) = C_1\left(x,t,D_1,C_{sat,1}\right) + C_2\left(x,t,D_2,C_{sat,2}\right) \tag{2}$$

where

$$C_\infty = C_{sat,1} + C_{sat,2} \tag{3}$$

978-1-4673-1965-2/12/$31.00 ©2012 IEEE

C_∞ is the total saturated moisture concentration. As long as the parameters of $D_1, C_{sat,1}$ and $D_2, C_{sat,2}$ are known from experiments, the non-Fickian behavior can be solved by two separate Fickian diffusions using finite element analysis.

For subsequent desorption analysis, if there is a permanent residual moisture in material, it is reasonable to assume that $C_2 = C_r$ (constant) with $D_2 = 0$, indicating the bound water will not be removed from the material. In this case, Equation (2) becomes

$$C(x,t) = C_1(x,t,D_1,C_{sat,1}) + C_r \tag{4}$$

It is noted that in Equation (4), if C_r is known, equation (4) becomes a single-stage Fickian-type diffusion, so-called modified Fickian diffusion model in [4,11].

Desorption at a higher temperature may remove the bound water completely. In this case, Cr = 0 in Equation (4). A Fickian diffusion process may then be assumed.

3. Diffusion Material Properties

The moisture absorption and desorption behavior of the epoxy molding compound (EMC) samples were studied experimentally [5]. The EMC samples of 1 mm thick with a 50 mm diameter disk were tested at 85°C /85% RH for 10 days, then subjected to 85°C /0% RH desorption for 12 days. The dual stage fit for both absorption and desorption are shown in Figure 1, and Table 1 list the values of diffusivity and moisture concentration for both absorption and desorption. Several important observations are made: 1) non-Fickian diffusion is much slower than Fickian diffusion, which is reflected from the values of D_1 and D_2. 2) The non-Fickian moisture diffusion contributes to about 25% of the Fickian saturated moisture concentration ($C_{sat,2}/\ C_{sat,1}$). This portion of moisture absorption is nonreversible during desorption process. The dual-stage fitted data match the residual moisture concentration measurement well. 3) Fickian diffusivity for absorption and desorption are obtained by fitting the experimental data separately. The results confirm that the Fickian diffusivity is same at both absorption and desorption, indicating the first stage is completely reversible. The results also show the Fickian saturated moisture concentration in absorption equals to the saturated moisture absorption at desorption.

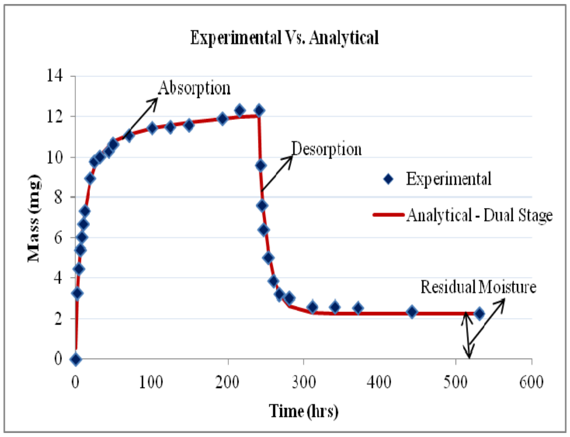

Figure 1 Dual stage fit - absorption

Table 1 Dual stage parameters

	Absorption	Desorption
D_1 (mm^2/hr)	8.00E-03	8.00E-03
C_{sat1} (mg/mm^3)	5.00E-03	5.00E-03
D_2 (mm^2/hr)	8.50E-04	0
C_{sat2} (mg/mm^3)	1.27E-03	1.15E-03

Experimental results for desorption at elevated temperatures using an in-situ moisture analyzer show that the moisture diffusion follows a Fickian characteristic well [5]. Figure 2 shows the reproduced desorption data over an extended period of time using Fickian desorption parameters in Table 2. Higher temperature corresponds to less percentage of the permanent residual moisture content in material. At 120°C, 90% of the initial moisture for all samples is diffused out within 24 hours as shown in Figure 2. Longer exposure time result in all the residual moisture removed from the sample. This supports the previous study by Zhou et al. [3] that higher temperature and longer exposure time is required to remove the permanent residual or Type II bond water molecules.

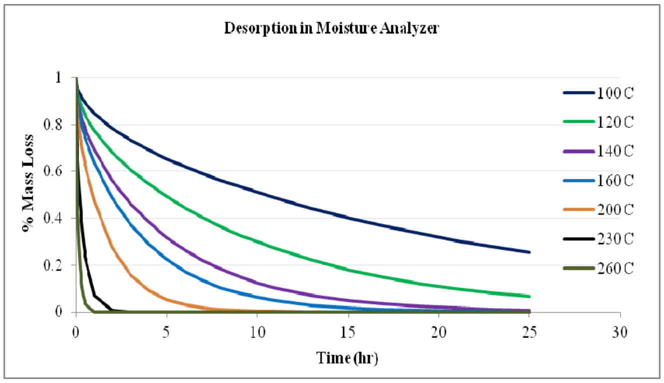

Figure 2 Desorption results at various temperatures for a mold compound

Table 2. Fickian desorption parameters at various temperature

Temperature (°C)	D (mm^2/hr)	Csat (mg/mm^3)
100	5.78E-03	6.27E-03
120	1.24E-02	
140	2.31E-02	
160	3.18E-02	
200	6.71E-02	
230	3.11E-01	
260	7.32E-01	

4. Finite Element Modeling

When Fick's Law is used, the transient moisture diffusion is governed by a similar governing differential equation used for transient heat transfer analysis. Galloway et al. [7] have demonstrated that the commercially available finite element software for transient heat analysis can be effectively used for transient moisture diffusion modeling. For a non-Fickian moisture diffusion process, two separate Fickian diffusion analyses are performed first using the dual-stage model parameters. A single script with ANSYS APDL is developed to perform the anomalous moisture diffusion automatically. If a desorption process is followed, and the residual moisture content is considered, the script can continuously perform the diffusion modeling correctly. As an example, a two dimensional finite element simulation to characterize the dual stage moisture absorption and desorption of a thin plate sheet of dimension 50mm x 1mm is conducted. Figure 3 shows the comparison between finite element results and analytical model results in terms of the total mass of moisture content as function of time. It shows the approach can simulate the anomalous moisture diffusion during absorption and also take considerations of the residual moisture effect during desorption process. Figure 4 shows the analytical and the finite element simulation results for moisture concentration at the middle plane for 85°C/85%RH absorption followed by 85°C/0%RH desorption. Again, the excellent agreement has been made.

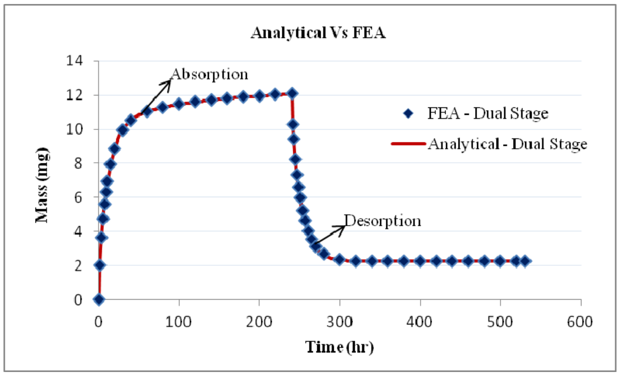

Figure 3 Mass gain and loss - 85°C/85%RH absorption and 85°C/0%RH desorption

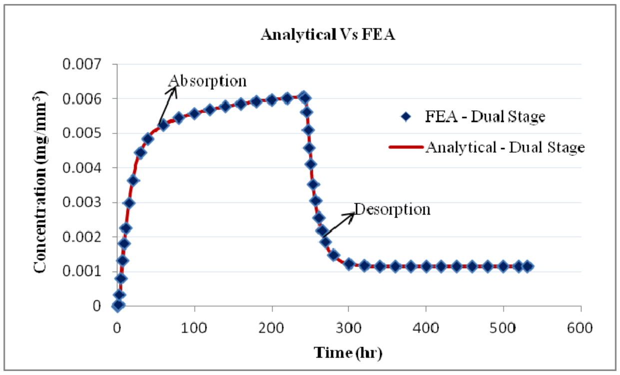

Figure 4 Moisture concentration - 85°C/85%RH absorption, 85°C/0%RH desorption

This work is extended to simulate a process that includes moisture absorption at 85°C/85%RH, and then a reflow process. The simplified profile is as shown in Figure 5 to define the temperature change during reflow. The diffusive properties in Table 2 are used. The process starts from a dual-stage non-Fickian moisture diffusion at 85°C/85%RH for a duration of 240 hours. Then the reflow process of about 300 seconds (5 minutes) is followed, using Fickian diffusion analysis as shown in Figure 2. A single script is used for the whole process. Figure 6 shows the mass loss as function of time at reflow. The finite element simulation results are validated by comparing with the analytical results. Results show that about 80% of the total moisture is desorbed during the reflow duration of less than 5 minutes.

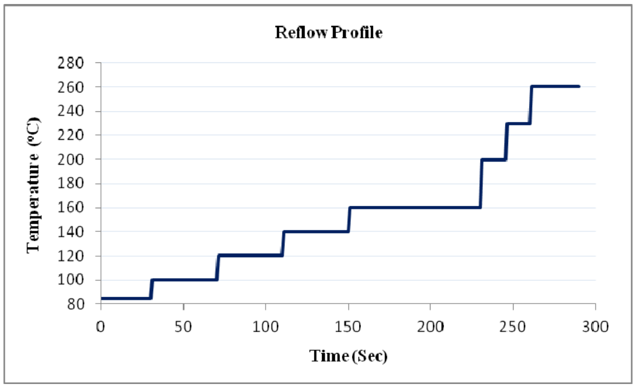

Figure 5 Reflow profile for the desorption simulation

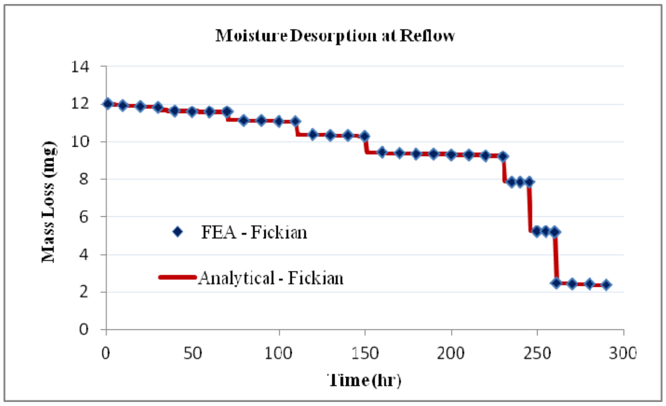

Figure 6 Moisture loss during reflow

5. Conclusions

Using a dual-stage model with both stages described by Fickian terms mathematically, this paper presents the finite element results of anomalous moisture diffusion using commercial finite element analysis software. ANSYS script is developed to run a single analysis to obtain the results for the whole process including absorption and desorption phases. The results are validated by the analytical and experimental results. The future work will extend the approach to multi-material system in a reflow process.

References

1. Fan XJ, Suhir E. Moisture Sensitivity of Plastic Packages in IC Devices. Springer, New York 2010.
2. Fan XJ, Lee SWR, Han Q. Experimental investigations and model of study of moisture behaviors in polymeric materials. *Microelectronics Reliability* 2009;49:861-871.

3. Zhou J, Lucas JP. Hygrothermal effects of epoxy resin. Part I: the nature of water in epoxy. *Polymer* 1999;40(20):5505-5512.
4. Placette MD, Fan XJ, Zhao JH, Edwards D. A dual stage model of anomalous moisture diffusion and desorption in epoxy mold compounds. Proc. 12th. Int. Conf. on Thermal Mechanical and Multiphysics Simulation and Experiments in Micro-Electronics and Micro-Systems (EuroSimE) 2011.
5. Fan XJ, Nagaraj V. Experimental characteristics of moisture absorption and desorption in conductive adhesives and epoxy mold compounds. Proc. 12th. Int. Conf. on Thermal Mechanical and Multiphysics Simulation and Experiments in Micro-Electronics and Micro-Systems (EuroSimE) 2012.
6. Tay AAO, Lin TY. Moisture diffusion and heat transfer in plastic IC packages. IEEE Transactions on components, packaging and Manufacturing Technology, Part A. 1996;20(3):186-193.
7. Galloway JE, Miles BM. Moisture absorption and desorption predictions for plastic ball grid array packages. IEEE Trans. Compon. Packag. Manuf. Technol. 1997;20(3):274-279.
8. Wong EH, Teo YC, Lim TB. Moisture diffusion and vapor pressure modeling of IC packaging. Proceedings of the 48th Electronic Components and Technology Conference. 1998:1372-1378.
9. Xie B, Fan XJ, Shi XQ, Han D. Direct concentration approach of moisture diffusion and whole field vapor pressure modeling for reflow process: part I-theory and numerical implementation. ASME J.Electron. Packag. 2009;131:031010-7.
10. Xie B, Fan XJ, Shi XQ, Han D. Direct concentration approach of moisture diffusion and whole field vapor pressure modeling for reflow process: part II-application to 3D ultrathin stacked-die chip scale packages. ASME J. Electron. Packag. 2009;131: 031011-6.
11. Placette MD, Fan XJ, Zhao JH, Edwards D. Dual stage modeling of moisture diffusion and desorption in epoxy mold compounds. Microelectronics Reliability 2012:(to appear).
12. Carter HG, Kibler KG. Langmuir-type model for moisture diffusion in composite resins. Journal of Composite Materials 1978;12:118-131.
13. Gurtin ME, Yatomi C. On a model for two phase diffusion in composite materials. 1978;13:126-130.