

A Note on the Normalized Approach to Simulating Moisture Diffusion in a Multimaterial System Under Transient Thermal Conditions Using ANSYS 14 and 14.5

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Moisture can have significant effects on the performance and reliability of electronic components. Accurately simulating moisture diffusion is important for designers and manufacturers to obtain a realistic reliability evaluation. Beginning with version 14, ANSYS is capable of simulating diffusion and related behaviors, such as hygroscopic swelling, with newly developed elements. However, a normalized approach is still required to deal with the discontinuity of concentrations at the material boundaries, and normalization of the moisture concentration in transient thermal conditions is tricky. Case studies have shown that normalizing the moisture concentration with respect to a time- or temperature-dependent material property will lead to erroneous results. This paper re-addresses the issues of performing diffusion simulations under transient thermal conditions and more general anisothermal conditions (temporally and spatially), and suggests an easy-to-use approach to cope with the limitations of the current version for users in the electronic packaging industry.

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1 Prior Arts on Moisture Diffusion Simulation With Normalized Approach

Moisture-related failure, such as the notorious popcorn failure during reflow soldering, is an important failure type for electronic components. Numerous researchers have been engaged in moisture-related research activities, such as measuring the diffusivity, solubility [1,2], and coefficient of hygroscopic swelling (CHS) [3–5], and studying the failure mechanisms [6,7]. In recent years, computational methods have been used to determine the amount, distribution, and subsequent effects of moisture. The moisture diffusion process can be simulated using appropriate numerical approaches, such as the finite element method (FEM); and moisture-induced issues such as stress and deformation can be analyzed for further evaluation of the packaging reliability. Commercial finite element software packages, which can handle coupled-field simulation in complex structures with different materials, have been widely used.

Two tasks must be accomplished for accurately simulating the moisture diffusion in a system containing two or more materials. The first task is to implement the diffusion equations numerically,

and the second is to properly handle the moisture concentration and flow at the interface of the two different materials. Prior to the release of ANSYS 14, a widely used method adopted by ANSYS users to fulfill the first task was to use thermal analogy based on the similarity of the governing equations of heat transfer and moisture diffusion [8,9]. For heat transfer, the diffusion equation gives

$$\rho c_p \dot{T} = \nabla \cdot (k \nabla T) \quad (1)$$

where ρ is the density, c_p is the specific heat, T is the temperature, and k is the thermal conductivity. And for moisture diffusion, Fick's second law gives

$$\dot{C} = \nabla \cdot (D \nabla C) \quad (2)$$

where C is the concentration and D is the moisture diffusivity. The similarity between Eqs. (1) and (2) is so obvious that a direct analogy can be easily formulated [8]. For ANSYS 14 and 14.5, the moisture diffusion process can be directly simulated using corresponding elements, and coupled-field simulations with heat transfer and structural analyses can be achieved simultaneously [10,11].

The second issue is usually handled by using a normalized approach. At a given temperature, the moisture concentration at the material interface follows the Nernst distribution law

$$\chi = \frac{C_{\text{Mat1}}}{C_{\text{Mat2}}} = \frac{C_{\text{sat1}}}{C_{\text{sat2}}} = \text{const} \quad (3)$$

where C_{Mat1} and C_{Mat2} are the concentrations of two materials at the interface, and C_{sat1} and C_{sat2} are the saturated concentrations of those two materials. Therefore, the discontinuity can be handled by introducing a normalized field variable,

$$w = C / C_{\text{sat}} \quad (4)$$

Because $C_{\text{sat}} = SP_{\text{VP}}$, where S is the solubility and P_{VP} is the ambient vapor pressure of the environment, an alternative way is to define,

$$\phi = C / S \quad (5)$$

as the normalized concentration, and in this case, the ambient vapor pressure P_{VP} is treated as a boundary condition. By substituting concentration C with $S\phi$ in Eq. (2), Fick's law in terms of normalized concentration yields

$$\dot{S}\phi + S\dot{\phi} = \nabla \cdot [D \nabla (S\phi)] \quad (6)$$

From a practical point of view, for most problems in the packaging area, we may neglect the effect of the spatial temperature gradient and consider the solubility to be uniform for each material, since the spatial temperature difference is usually not large enough to affect the diffusion parameters in this particular research area. Based on this assumption, the diffusion equation for each material can be simplified as

$$\dot{S}\phi + S\dot{\phi} = \nabla \cdot (DS \nabla \phi) \quad (7)$$

Similarly, if another normalization method is adopted (such as using saturated concentration C_{sat}), Eqs. (6) and (7) will still hold, except that the solubility S should be replaced by the corresponding material property.

The solubility can be expressed as

$$S = S_0 \exp\left(\frac{E_s}{RT}\right) \quad (8)$$

where E_s is the activation energy for solubility, S_0 is a material property, and R is the gas constant. It is very clear that $\dot{S} = 0$

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under isothermal conditions (temporally and spatially, i.e., $\dot{T} = 0$ and $\nabla T = 0$), so that Eq. (7) can be rewritten as

$$S\dot{\phi} = \nabla \cdot (DS\nabla\phi) \quad (9)$$

Another analogy scheme, referred to as the “normalized analogy,” can be formulated based on Eqs. (1) and (9). This approach is suitable for diffusion problems in multimaterial systems under isothermal conditions, for example, the moisture ingress into electronic components encapsulated by the molding compound in the 85/85 or HAST test. However, it has been pointed out that this normalization method may lead to incorrect results under transient thermal conditions ($\dot{T} \neq 0$), or more general temporally and spatially anisothermal conditions ($\dot{T} \neq 0$ and $\nabla T \neq 0$) [8,9,12]. For transient thermal conditions, since the solubility is a function of temperature, and ultimately a function of time, dropping the term $S\dot{\phi}$ would lead to erroneous results, and, unfortunately, this is the limitation of the normalized analogy. The same issue arises if we normalize the moisture concentration with respect to the saturated concentration instead of solubility. For the saturated concentration,

$$C_{\text{sat}} = SP_{\text{VP}} = S \times P_{\text{sat}} \times \text{RH} \quad (10)$$

and

$$P_{\text{sat}} = P_0 \exp\left(-\frac{E_{\text{VP}}}{RT}\right) \quad (11)$$

where E_{VP} is the activation energy for vapor pressure and RH represents relative humidity. Hence,

$$C_{\text{sat}} = S_0 P_0 \exp\left(\frac{E_s - E_{\text{VP}}}{RT}\right) \times \text{RH} \quad (12)$$

We may see that there is no guarantee that C_{sat} is independent of time, so performing normalization with respect to C_{sat} is not suitable for transient thermal conditions, either. In other words, there is no way to further simplify Eq. (7) in transient thermal cases, unless the normalized concentration can be defined as the concentration divided by a time- and temperature-independent material property. Based on the results of the experimental measurement, that is $E_s \approx E_{\text{VP}}$ for many electronic packaging materials [2], Jang et al. defined that property as [9]

$$M = S_0 P_0 \quad (13)$$

and defined

$$\phi = C/M \quad (14)$$

as the new normalized concentration. Obviously, M is a temperature-independent material property. Therefore, Eq. (7) can be simplified to a form similar to Eq. (9), with the solubility S replaced with M , which is referred to as the “modified solubility.” This analogy scheme is named the “advanced analogy,” and in contrast, the normalization method using the solubility or saturated concentration is referred to as the “conventional” method by Jang et al. The comparison between the simulation results of the different methods is shown in Ref. [9].

2 Issues in Simulation With ANSYS 14.5

ANSYS adopted the normalized approach in its diffusion elements² (and coupled-field elements with diffusion capability³) to

²PLANE238, SOLID239, and SOLID240 (version 14.5 or later).

³PLANE223, SOLID226, and SOLID227 (version 14 or later).

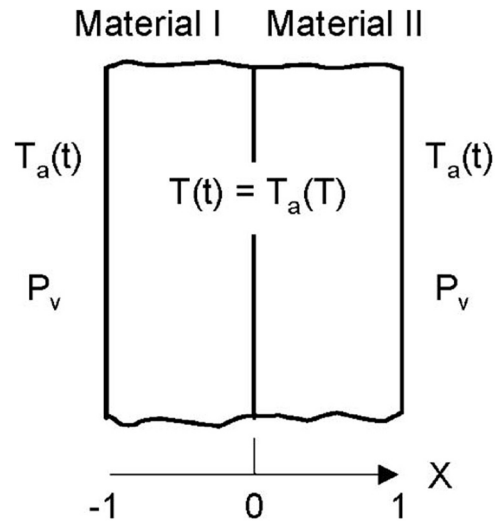


Fig. 1 Geometry and boundary conditions for the case study ($T_a = 25 + t/60$ °C, $P_v = 3207$ Pa)

handle the discontinuity issue at the material boundaries. The ANSYS theory reference provides a governing equation

$$\frac{\partial(C_{\text{sat}}\bar{C})}{\partial t} = C_{\text{sat}}[D]\nabla^2\bar{C} \quad (15)$$

where $\bar{C} = C/C_{\text{sat}}$ is the normalized concentration [11]. This equation, mathematically, has the same form as Eq. (7), with the only difference being notation. The “saturated concentration” is input as a material property (MPDATA, CSAT), and the ANSYS parametric design language allows this property to be input as temperature-dependent [11]. Apparently, other normalization methods can be implemented by simply inputting the corresponding properties (such as solubility S or modified solubility M) as the “CSAT” property in the material model.

Equation (15) is obviously correct; however, the method of handling this equation may lead to incorrect results. If the “saturated concentration” (CSAT) is simply updated step by step, then the effect of the rate change (\dot{C}_{sat} or \dot{S}) will not be included in the calculation, repeating the erroneous results as in the analogy method.

However, there is no example of temperature-dependent saturation in the documentation of ANSYS. Therefore, we performed a case study using the identical transient thermal problem as in Ref. [9]. The geometry of the model is shown in Fig. 1, and the material properties are summarized in Table 1. The temperature increased 1 °C per minute from the room temperature, while the vapor pressure was set at 3207 Pa (saturated vapor pressure at 25 °C), and kept constant during the heating process.

Two normalization methods were compared, one is a “conventional” normalization method with respect to the solubility S , and the other is the advanced normalization approach. For the latter case, a temperature-dependent boundary condition should be applied [9]

$$\phi_{\text{BC}}(t) = \frac{C(t)}{M} = \frac{S(t)P_v}{M} = \frac{S_0 P_v}{M} \exp\left[\frac{E_s}{RT(t)}\right] \quad (16)$$

Table 1 Material properties for analysis cases

	Material I	Material II
$D_0(\text{m}^2 \text{s}^{-1})$	5×10^{-3}	4×10^{-3}
$S_0(\text{kgm}^{-3} \text{Pa}^{-1})$	6×10^{-10}	2×10^{-10}
$E_D(\text{J mol}^{-1})$	5×10^4	5×10^4
$E_S(\text{J mol}^{-1})$	4×10^4	4×10^4

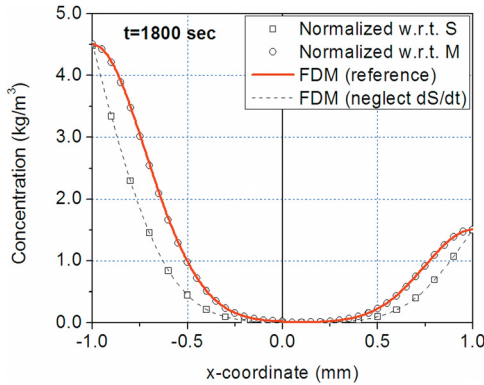


Fig. 2 Moisture concentration in a bimaterial specimen subject to transient loading conditions ($t = 1800$ s)

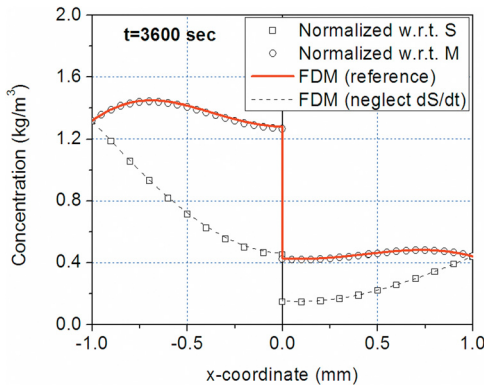


Fig. 3 Moisture concentration in a bimaterial specimen subject to transient loading conditions ($t = 3600$ s)

An eight-node diffusion element (PLANE238) was used for the finite element simulation. A program written using the finite difference method (FDM) was also used for verification, and the algorithm is described in detail in Ref. [8].

From the simulation results in Figs. 2 and 3, it is easy to see that different normalization methods give different results. The results from the “conventional” normalization method deviate significantly from the reference values. Actually, the incorrect results in Fig. 5 of Ref. [9] are repeated. The normalized approach using modified solubility (M) gives the same results as the FDM calculation, and the values agree with prior simulation results in Ref. [9].

To illustrate the root of the erroneous results, we forced \dot{S} to be zero in the FDM program to intentionally generate a “wrong” solution, and the data matched the incorrect FEM results perfectly. Clearly, the effect of the rate of change of the “CSAT” property was omitted by the program, and, therefore, the “saturated concentration” property in ANSYS (MPDATA, CSAT) must not be temperature-dependent for simulations in transient thermal conditions, otherwise, the result would be inaccurate due to this flaw. As a result, performing simulation in such conditions becomes very tricky. A more complicated “truly anisothermal” case ($\dot{T} \neq 0$ and $\nabla T \neq 0$) is not covered in this paper, since the conclusion will be evident [9].

3 Summary and Discussion

Our case study has indicated that for a multimaterial system under transient thermal conditions, the simulation result using

current versions of ANSYS is dependent on the normalization method. The newly developed diffusion elements behave similarly to the thermal elements; however, the differences between the transient thermal simulation and moisture diffusion simulation are apparent. For the thermal analysis of solid materials, the temperature dependency of density ρ and specific heat c_p could be very weak; however, for the moisture diffusion analysis, the solubility changes exponentially with the temperature. Using a temperature-dependent material property for normalization will lead to erroneous results in the moisture diffusion analysis. Although the analogy method is no longer needed for ANSYS users after the release of version 14, the accumulated knowledge about normalization methods is still valuable.

It is worth mentioning that besides the normalized approach, researchers such as Xie et al. have also developed a direct concentration approach (DCA) [12]. Unlike Jang’s approach, which utilized the approximate equivalence of the activation energy for vapor pressure and solubility, DCA does not rely on the relationship between such properties, and has a potentially larger field for application. The DCA has been implemented using ABAQUS, studying the moisture-related issues during the reflow process [13]. However, for packaging materials with $E_s \approx E_{VP}$, the normalization method proposed by Jang et al. [9] appears to be simpler, especially for users of ANSYS 14 or later versions.

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