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# Predicting non-Fickian moisture diffusion in EMCs for application in micro-electronic devices

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ABSTRACT

This study made an attempt to predict the temperature-dependent moisture diffusion of an epoxy molding compound with 3 different diffusion models: Fickian, dual stage and Langmuir diffusion. The Langmuir model provided the best prediction of the moisture diffusion when simulating the input experiments. Beyond the temperature range of the input experiments, the Langmuir model was still able to provide a fair prediction. Hence, the Langmuir model also provides better predictions for the moisture distribution in general. This allows for building on existing prediction models and enabling simulations of reliability tests like UHST.



## 1. Introduction

Most electronic devices are encapsulated with epoxy molding compound (EMC) to protect the device: protecting the design by making the device invisible, protecting very small structures in a mechanical sense by putting them in a supporting matrix, and protecting the electronic components against moisture and thereby against corrosion and electrical breakdown.

EMC is essentially a silica-filled polymer network. It is not a perfect moisture barrier, as it still takes up a small amount of water despite being filled with up to 90% by weight of the fillers. The moisture uptake is so low that, during normal use and service life, it only leads to a slow degradation of the electronic device especially if the package is robust enough to resist ingress of moisture from the outside of the package due to delamination or cracks. To test the resistance of the device to corrosion accelerated tests like HAST (Highly Accelerated Stress test, usually under bias) are performed.

Popcorn cracking is a moisture-induced device failure. It is caused by moisture diffusion and uptake. During solder reflow, an intense pressure build-up is generated by the vaporization of the internal moisture. This pressure leads to failure of a device interface or 'blows up' the device. A popping sound may actually be heard at the moment of fracture of the device-EMC interface. This effect is not seen with devices which are dry-baked prior to the solder reflow. Although popcorn cracking will hardly ever occur during normal service life, as the temperature ramps are most often not so extreme, it can be used as a measure of the robustness of the device.

As mentioned, the robustness of an electronic device is currently tested by actual accelerated tests. However it would be very valuable to simulate such tests during the design phase, which will improve the time-to-market and reduce development costs. However, to model reflow tests, accelerated stress tests and phenomena like popcorn cracking, accurate prediction of moisture diffusion and distribution are required.

A lot of work has already been done on the predictive modeling of moisture diffusion in EMCs and in electronic devices [1–6]. Some workers have even tried to simulate popcorn cracking [7]. In most cases, diffusion is assumed to follow Fick's laws. However, our own experiments have shown that moisture diffusion in EMCs do not always follow Fickian behavior as also reported by other workers [8]; instead of reaching a constant level of saturation (after many hours) it seems that a constant rate of moisture intake is reached. Hence, the moisture uptake curve ends with a constant slope instead of a constant value (zero slope). For reasons of simplicity, this more complicated behavior is simplified to standard Fickian behavior. This standard Fickian behavior can be implemented easily within most finite element codes by using the analogy between thermal and moisture diffusion [9]. Nevertheless, this induces errors, making it less valuable under certain circumstances [10].

Therefore, the aim of this study was to fit moisture diffusion experiments with both Fickian and non-Fickian models. The diffusion models which were used were: Fickian, dual stage [11,12] and Langmuir diffusion [13]. The models were also implemented within finite element

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software to make them applicable for predictive simulations. The model fits were verified with UHST (Unbiased Highly Accelerated Stress Test) experiments. UHST is an accelerated moisture test that is performed under 130 °C/85% RH. The ability to predict the kinetics of moisture diffusion under these relatively extreme conditions would improve our understanding of failure mechanisms like bond pad corrosion, for example.

## 2. Materials and methods

### 2.1. Model generation

The EMC used in this study was a typical biphenyl epoxy molding compound. Absorption experiments were performed on EMC test samples of 90.0 × 4.5 × 2.0 mm$^3$. The test conditions are described in Table 1. These experiments were performed in a climate chamber, and the samples were weighed at different readpoints during the experiment.

From earlier experience, it is known that the amount of samples is sufficient to obtain a reliable result. Furthermore, when the samples are weighed, they are removed from the climate chamber. During this period, the sample desorp/dry, affecting the result of the experiment. A larger amount of samples leads to a too long period outside the climate chamber.

Each absorption test was fitted with the three different diffusion models: 3-dimensional Fickian diffusion, dual stage diffusion and Langmuir diffusion. The obtained model parameters were: diffusion coefficient, saturated concentration and the Langmuir parameters. These are only valid at the temperature at which the experiment is performed, which was constant. However, the experiments were performed at different temperatures. Therefore, the obtained model parameters from all experiments were fitted into a temperature dependent model for Fickian, dual stage and Langmuir diffusion.

### 2.2. Implementation and verification

The models were implemented within finite element (FE) code (MSC.MARC) and absorption experiments were performed by weighing the samples successively after exposure to different MSL conditions (Table 1). Another four absorption experiments were performed to verify whether the temperature dependent models and the implementation are also valid beyond the initial experiments which were used to generate the model parameters. Therefore it was decided to perform the UHST just below and just above the glass temperature of the EMC. UHST experiments were performed on test samples of 90.0 × 4.5 × 2.0 mm$^3$ (Table 2).

## 3. Theory

### 3.1. Fickian diffusion model

Transient Fickian (isotropic) moisture diffusion can be described with

$$\frac{\partial C}{\partial t} = D\Delta C \qquad (1)$$

**Table 1**
Test conditions (*: 2nd dataset done at a different time period).

| Test conditions | Testing period (h) | Amount of samples |
|---|---|---|
| 30 °C/60%RH (MSL3) | 600 | 4 |
| 30 °C/60%RH (MSL3)* | 1585 | 4 |
| 60 °C/60%RH | 2382 | 4 |
| 85 °C/85%RH (MSL1) | 336 | 4 |

**Table 2**
UHST test conditions (verification).

| Test conditions | Testing period (h) | Type of sample | Amount of samples |
|---|---|---|---|
| 110 °C/85%RH | 40 | 90.0 × 4.5 × 2.0 mm$^3$ | 2 |
| 110 °C/85%RH | 191.5 | 90.0 × 4.5 × 2.0 mm$^3$ | 2 |
| 130 °C/85%RH | 44 | 90.0 × 4.5 × 2.0 mm$^3$ | 3 |

$$w = \frac{C}{C_{sat}(\%\mathrm{RH}, T)} \qquad (2)$$

where C is a concentration (kg/m$^3$), D a diffusion coefficient (m$^2$/s), $C_{sat}$ a saturated concentration (kg/m$^3$) and w a wetness. The wetness is a dimensionless parameter which is assumed to be constant at an interface of two moisture sensitive materials. The solution for the 3D situation is:

$$\frac{M_t}{M_{sat}} = 1 - \left(\frac{8}{\pi^2}\right)^3 \sum_{K=0}^{\infty}\sum_{L=0}^{\infty}\sum_{M=0}^{\infty}\cdots \frac{1}{K^2 \cdot L^2 \cdot M^2} e^{-\left(\frac{D_x K^2}{x^2}+\frac{D_y L^2}{y^2}+\frac{D_z M^2}{z^2}\right)\cdot t\cdot\pi^2}. \qquad (3)$$

### 3.2. Dual stage or dual phase diffusion model

The dual stage model is a combination of two Fickian diffusion models with different parameters. Both these Fickian models are completely independent of each other. Hence, the total moisture distribution ($C_{total}$) within a material is made up of two separate/distinct moisture concentrations ($C_1$ and $C_2$). The change of concentration $C_1$ depends on diffusion coefficient $D_1$ and the change of concentration $C_2$ depends on diffusion coefficient $D_2$. There is no flow between concentrations $C_1$ and $C_2$. The dual stage diffusion model is an empirical model which does not reflect or represent actual physics.

### 3.3. Langmuir diffusion model

This model was presented by Carter et al. [13] and the authors suggested that moisture diffusion could just as well follow Kirkwood's (linear) generalization of the Boltzmann transport equation instead of the simple diffusion theory. The model involves sources and sinks of diffusing water molecules. With respect to diffusive characteristics, the model is related to the simplest form of neutron transport theory. With respect to bound and unbound particles it is similar to the Langmuir theory of adsorption isotherms.

Langmuir diffusion can be described with

$$\frac{\partial C_1}{\partial t} + \frac{\partial C_2}{\partial t} = D\Delta C_1 \qquad (4)$$

$$\frac{\partial C_2}{\partial t} = \alpha \cdot C_1(t) - \beta \cdot C_2(t). \qquad (5)$$

$C_1$ and $C_2$ are the concentrations of unbound and bound water, respectively. The 1D solution is:

$$\frac{M_t}{M_{sat}} = 1 - \frac{8}{\pi^2}\sum_{K=0}^{\infty}\frac{(r_1 \cdot e^{-r_2 \cdot t} - r_2 \cdot e^{-r_1 \cdot t})}{(2\cdot K+1)^2 \cdot (r_1 - r_2)} + \frac{8\cdot\delta\cdot\beta}{\pi^2\cdot(\alpha+\beta)}\sum_{K=0}^{\infty}\frac{(e^{-r_2 \cdot t} - e^{-r_1 \cdot t})}{(2\cdot K+1)^2\cdot(r_1 - r_2)} \qquad (6)$$

with

$$\delta = \frac{D}{l^2}\cdot\frac{\pi^2}{4} \qquad (7)$$