

Popcorn Cavity Pressure

C. Glenn Shirley

Abstract—Evolution of the moisture concentration profile and cavity pressure in response to sudden exposure to a reflow ambient is shown for the simplest model of a plastic package with cavity. Careful definition of boundary conditions, particularly of mass balance at the molding compound/cavity interface shows that a superposition of two classical solutions to the diffusion equation for a specific class of boundary condition is necessary. The boundary condition analysis also points the way to modeling cavity pressure correctly in more complicated and realistic cases. The zero cavity size limit of the analytical solution is interesting because it shows, contrary to common belief, that a cavity is not necessary for the existence of very high internal pressures to cause mechanical damage.

Index Terms—Plastic integrated circuit packaging, reliability.

I. INTRODUCTION

THE POPCORN mechanism of package damage in the solder reflow process of circuit board assembly has been well understood since the late 1980's (Fukuzawa et. al. [1], Kitano et al [2], Bhattacharyya et al [3]). Alpern and Lee [4] give an up-to-date description. The molding compound of a plastic integrated circuit package absorbs a surprisingly large amount of water if exposed to the humidity in a normal room ambient. Absorbed water driven from the molding compound during the reflow generates internal water vapor pressure, P , which causes mechanical damage to the package. Fukuzawa et. al. [1] gave a simple model in which the pressure causes delamination of molding compound over the die or lead frame pad. In the model cracking occurs when the maximum bending stress on the long edge of a die or pad given by

$$\sigma_{\max} = 6K \left(\frac{a}{t} \right)^2 P \quad (1)$$

exceeds the bending strength of the molding compound at the reflow temperature. In Eq. (1) K is a geometrical factor ($K \cong 0.05$ for a square pad), a is the length of the long side of the die, and t is the molding compound thickness over the die or the pad. At typical reflow temperatures ($\sim 215^\circ\text{C}$) the bending strength of molding compound is about 10 MPa (98.7 Atm) [2]. For molding compound thickness of 2 mm over a square die or pad 12 mm on a side, Eq. (1) gives 9 Atm as the pressure threshold of package damage, which is the typical threshold mentioned by Kitano et. al [2]. According to Eq. (1)

thicker packages and/or smaller dies or pads will increase the pressure damage threshold. Details of materials, processing, dimensions etc. will affect the precise value of the pressure damage threshold, but 9 Atm will be used for examples given in this paper.

Models of P consider moisture diffusion through the molding compound and into a delamination-induced internal cavity of the package (see Wong et al [5] for a recent review). A lack of consensus on how to approach modeling of pressure in cavities (see [5]) motivates the present paper. The strategy here is to analyze the simplest model of a package with a cavity which has the essential physics of internal pressure generation. Not covered are mechanisms by which this pressure drives package flexure, crack nucleation and growth, etc. Insight gained by focusing only on moisture transport suggests improvements to more realistic models.

The plan of the paper is as follows. In Section II properties of water vapor and molding compound are reviewed and an example preconditioning and reflow scenario used later in the paper is set up. In Section III a detailed one-dimensional model is described, first by careful derivation of boundary conditions, and then by writing down solutions which satisfy the boundary conditions. A key result is derivation of a boundary condition at the molding compound/cavity interface which relates the moisture concentration gradient there to the rate of change of moisture concentration there. In the first place this boundary condition points to a certain class of solutions to the diffusion equation in the standard catalog of solutions, [6]. In the second place, the boundary condition is all that is needed to compute the cavity pressure. Section IV shows the solution to the equations given in Section III for the conditions set up in Section II. The final section explains how cavity pressure can be modeled properly for more complicated and realistic cases.

II. PROPERTIES OF MOLDING COMPOUND AND WATER VAPOR

Molding compound absorbs moisture until it comes to equilibrium with the surrounding ambient containing water vapor. The equilibrium concentration of water in the molding compound is given by Henry's Law $\mu = SP$ where μ (mole/m³) is the saturated molar density of water in the molding compound, P (Pa) is the partial pressure of water vapor in the ambient and S is the solution coefficient given by

$$S = S_\infty \exp\left(\frac{Q_m}{RT}\right). \quad (2)$$

Kitano et al [2] give $S_\infty = 2.75 \times 10^{-8}$ mole/m³Pa and $Q_m = 38.7$ kJ/mole (0.401 eV). $R = 8.3145$ J/moleK is the

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universal gas constant and T is the absolute temperature in °K. The partial pressure of water vapor in an ambient at temperature T and relative humidity H is given by

$$P = HP_{sat}(T) \quad (3)$$

where P_{sat} is the saturated vapor pressure given in a good approximation by, for example, Shirley [7]. The molar concentration of water vapor ρ (mole/m³) in the ambient is given by Boyle's law,

$$\rho = P / RT. \quad (4)$$

The result of exposure to a humid ambient can be gauged by the ratio $\mu/\rho = SRT$ from Boyle's and Henry's laws. At room temperature (25°C) $\mu/\rho = 413$ showing the large amount of water which can be absorbed in room ambients, given sufficient time.

The rate at which moisture comes to an equilibrium spatial distribution is governed by Fick's laws of diffusion which are (in one dimension)

$$D \frac{\partial \mu}{\partial x} = -J \quad \frac{\partial \mu}{\partial t} = D \frac{\partial^2 \mu}{\partial x^2} \quad (5)$$

where x (m) and t (s) are position and time, D (m²/s) is the diffusivity of moisture in the molding compound, and J is the flux (mole/m²s). Kitano et al [2] give the moisture diffusivity as

$$D = D_{\infty} \exp\left(-\frac{Q_d}{RT}\right) \quad (6)$$

where $D_{\infty} = 4.72 \times 10^{-5}$ m²/s and $Q_d = 48.4$ kJ/mole (0.502 eV).

The latent heat of vaporization of water, $Q_{lv} = 40.7$ kJ/mole (0.42 eV), is a measure of the strength of hydrogen bonding of water molecules in the liquid phase. The similar value of Q_m (0.401 eV) and the highly hygroscopic nature of absorption of water into molding compound suggests the same bonding mechanism of water to the organic molecules of the molding compound. On the other hand, the activation energy of diffusion of water through molding compound Q_d (0.502 eV) is a measure of the potential barriers that water molecules must surmount to move through the solid state, and is quite different from the activation energy of self-diffusion in liquid water (0.18 eV). The self-diffusivity of water is $D_{water} = D_{water,\infty} \exp(-Q_{water}/kT)$ where $Q_{water} = 0.18$ eV and $D_{water,\infty} = 2.65 \times 10^{-6}$ m²/s [8]. Diffusion in molding compound ranges from four orders of magnitude slower than liquid water at room temperature to two orders of magnitude slower at 200°C.

Thermal diffusion in molding compound is also governed by Fick's laws with thermal diffusivity

$$\kappa = \frac{K}{C_p \rho} = \frac{0.8 \text{ W.m}^{-1} \text{ K}^{-1}}{1052 \text{ J.kg}^{-1} \text{ K}^{-1} 1800 \text{ kg.m}^{-3}} = 4.22 \times 10^{-7} \text{ m}^2 \text{ s}^{-1} \quad (7)$$

where constants from Tay and Lin [9] have been used.

Sensitivity of packages to the popcorn mechanism is tested using, for example, the IPC/JEDEC moisture/reflow

sensitivity classification method [10]. First, the package is exposed to a "preconditioning" ambient (eg. 168 h at 85°C and 85% RH) to establish a spatially uniform equilibrium moisture concentration in the molding compound. Next, the package is placed in a "reflow" ambient and is subjected to increasing temperatures culminating in exposure to a peak temperature (eg. 215°C) for less than 20 seconds (for Pb-based technology). The gas of the reflow ambient is typically dry forming gas (nitrogen with a few percent H₂) with negligible moisture content. The IPC/JEDEC preconditioning and reflow ambients were simplified to the conditions in Table I. The "reflow" condition in Table I mimics the "peak package body temperature" in the IPC/JEDEC method [10] for which the duration must not exceed 20 seconds. The relative humidity, H , of the reflow ambient in Table I was set to an arbitrary plausible low value (0.1%) since the precise value does not affect the results. The very large change of μ between the preconditioning ambient and the reflow ambient seen in Table I is the driving force for the popcorn mechanism. Notice also that D is at least 3 orders of magnitude less than κ so thermal equilibrium is reached instantly compared to moisture transport equilibrium.

TABLE I MOLDING COMPOUND AND WATER VAPOR PROPERTIES AT EQUILIBRIUM IN THE PRECONDITIONING AND THE REFLOW AMBIENT.

Property	Ambient		Units
	Preconditioning (0)	Reflow (1)	
T	85	215	°C
H	85	0.10	%
P_{sat}	0.571	20.8	Atm
P	0.485	0.021	Atm
μ	599	0.805	mole/m ³
ρ	16.5	0.519	mole/m ³
D	4.10×10^{-12}	3.12×10^{-10}	m ² /s
κ	4.22×10^{-7}	4.22×10^{-7}	m ² /s

The conditions in Table I are referred to in the model derived in the next section by the subscript "0" for Preconditioning and "1" for Reflow.

III. ONE-DIMENSIONAL MODEL

The simplest one-dimensional model of a plastic package with a cavity is shown in Figure 1. A slab of molding compound of thickness w is separated from an impermeable surface, such as the lead frame pad or die, by a cavity of width l . The outer surface of a package corresponds to the interface between the molding compound and the external ambient at $x = 0$, and the interface between the molding compound and an internal cavity is at $x = w$. The whole system has an indefinitely large area A , corresponding to the die or pad area. The cavity ambient is isolated from the external ambient and can only come to equilibrium with it by diffusion through the molding compound.

Suppose the system in Figure 1 is exposed to the preconditioning ambient long enough to reach equilibrium. That is, the temperature and humidity of the system are held at T_0 and H_0 for a long time so that μ and ρ settle at values μ_0 and ρ_0 given by the "preconditioning column of Table I. The initial concentration profile is given by

$$\mu(x,0) = H_0 P_{sat}(T_0) S_0 \equiv \mu_0, \quad (0 \leq x \leq w, t=0) \quad (8)$$

Then, at $t=0$, the system is suddenly exposed to a reflow ambient with temperature T_1 and relative humidity H_1 . For $t > 0$ moisture diffuses out of the molding compound into the ambient and into the confined cavity, increasing the cavity moisture concentration and therefore the cavity pressure. If the package remains at the reflow condition eventually moisture concentration in the cavity falls to the equilibrium level corresponding to T_1 and H_1 by moisture diffusion through the molding compound to the external ambient thereby reducing the cavity pressure. The cavity pressure occurring in the transition from equilibrium at T_0 and H_0 to equilibrium at T_1 and H_1 is the driving force of the popcorn mechanism.

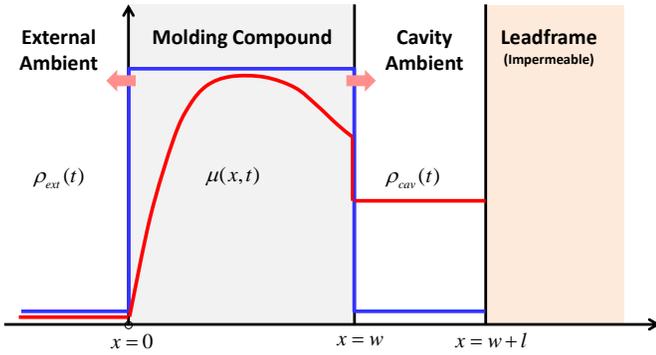


Figure 1. One-dimensional model of a plastic package with a cavity between molding compound and lead frame. The moisture concentration established by long exposure to the “preconditioning” ambient (blue) evolves after exposure to the reflow ambient (red). Moisture driven across the molding compound/cavity interface increases the cavity moisture concentration and the cavity pressure.

A. Boundary Conditions

Boundary conditions at the molding compound interfaces to the external and cavity ambients define the essential aspects of the mechanism. Henry’s law instantaneously relates molding compound surface concentrations to vapor pressures (and therefore, by Boyle’s law, vapor concentrations) in the external and cavity ambients.

At the molding compound/external ambient interface at all times after the step, Henry’s law requires that the surface moisture concentration of the molding compound be pinned at the constant value

$$\mu(0,t) = H_1 P_{sat}(T_1) S_1 \equiv \mu_1, \quad (x=0, t>0) \quad (9)$$

The external ambient concentration is also constant

$$\rho_{ext}(t) = H_1 P_{sat}(T_1) / RT_1, \quad (t>0) \quad (10)$$

At the molding compound/cavity ambient interface at all times following the step the molding compound surface concentration and the cavity concentration vary, but are related by Henry’s law

$$\mu(w,t) = RT_1 S_1 \rho_{cav}(t) \quad (x=w, t>0) \quad (11)$$

and, in particular, immediately after the step, the surface concentration at the molding compound/cavity surface is

$$\mu(w, t=0+) = RT_1 S_1 \rho_0 = \frac{T_1 S_1}{T_0 S_0} \mu_0 \quad (x=w, t=0+) \quad (12)$$

because the equilibrium cavity concentration established during preconditioning before the step is ρ_0 .

Mass balance is also a constraint at the molding compound/cavity interface because the rate of loss of moisture due to flux into the cavity at the interface given by Fick’s first law must equal the rate of increase in cavity moisture content. That is

$$-AD_1 \left. \frac{\partial \mu}{\partial x} \right|_{x=w} = JA = A \times l \frac{\partial \rho}{\partial t} \quad (\text{mole/s}) \quad (13)$$

where $A \times l$ is the volume of the cavity. Combining Eqs. (11) and (13) gives

$$\frac{\partial \mu}{\partial t} + h' \left. \frac{\partial \mu}{\partial x} \right|_{x=w} = 0 \quad (x=w, t>0) \quad (14)$$

where

$$h' = \frac{RT_1 S_1 D_1}{l}. \quad (15)$$

Eq. (14) is the condition which embodies the mechanism of cavity pressure and is an important result of this paper.

B. Solution of the Equations

It is convenient to write Eqs. (5), (8), (9), (12), and (14) in terms of the following (f , ε , and h are dimensionless)

$$m = \mu - \mu_0 \quad f = \frac{D_1 t}{w^2} \quad \varepsilon = \frac{x}{w} \quad h = RT_1 S_1 \frac{w}{l} \quad (16)$$

to give

$$\frac{\partial m}{\partial f} = \frac{\partial^2 m}{\partial \varepsilon^2} \quad (0 \leq \varepsilon \leq 1, f > 0) \quad (17)$$

$$m(\varepsilon, 0) = 0 \quad (0 \leq \varepsilon \leq 1, f = 0) \quad (18)$$

$$m(0, f) = a \quad (\varepsilon = 0, f > 0) \quad (19)$$

$$m(1, 0+) = b \quad (\varepsilon = 1, f = 0+) \quad (20)$$

$$\left. \frac{\partial m}{\partial f} + h \frac{\partial m}{\partial \varepsilon} \right|_{\varepsilon=1} = 0 \quad (\varepsilon = 1, f > 0) \quad (21)$$

where

$$a = \mu_1 - \mu_0 \quad b = \mu_0 \left(\frac{T_1 S_1}{T_0 S_0} - 1 \right). \quad (22)$$

VanSant [6] has cataloged many solutions to the diffusion equation in planar, cylindrical, and spherical geometries for many kinds of boundary conditions. The class of solutions with boundary conditions like Eq. (21) given by Carslaw and

Jaeger [11] are included. In particular, the solution to Eqs. (17) - (21) when $a = 1$ and $b = 0$ is solution 8.1.38 in VanSandt's catalog (or Eq. (9) on p129 of [11]):

$$m_a(\varepsilon, f, h) = 1 - \sum_{n=1}^{\infty} \frac{2(\gamma_n^2 + h^2) \sin(\gamma_n \varepsilon)}{\gamma_n (\gamma_n^2 + h^2 + h)} \exp(-\gamma_n^2 f). \quad (23)$$

And the solution to Eqs. (17) - (21) when $a = 0$ and $b = 1$ is solution 8.1.37 in VanSandt's catalog (or Eq. (8) on p128 of [11]):

$$m_b(\varepsilon, f, h) = \sum_{n=1}^{\infty} \frac{2h}{(\gamma_n^2 + h^2 + h)} \frac{\sin(\gamma_n \varepsilon)}{\sin(\gamma_n)} \exp(-\gamma_n^2 f). \quad (24)$$

In Eqs. (23) and (24) γ_n are the positive roots of $\gamma \tan \gamma = h$.

The series in the solutions in Eq. (23) and (24) do not converge rapidly at very short times ($f \ll 1$). The asymptotic solutions at short times may be found by recognizing that at short times the concentration profiles in the molding compound near the two interfaces do not interact. Carslaw and Jaeger give a well-behaved short-time solution of a semi-infinite slab of molding compound with boundary condition Eq. (19) (p305, Eq. (5), in [11]) and of a semi-infinite slab with boundary conditions Eqs. (20) and (21) (p306, Eq. (11), in [11]). For $f \ll 1$ the asymptotic forms of m_a and m_b are

$$m_a(\varepsilon, f, h) \sim \operatorname{erfc}\left(\frac{\varepsilon}{2\sqrt{f}}\right) \quad (25)$$

$$m_b(\varepsilon, f, h) \sim \exp\left[h(1-\varepsilon) + h^2 f\right] \operatorname{erfc}\left[\frac{1-\varepsilon}{2\sqrt{f}} + h\sqrt{f}\right]. \quad (26)$$

The solution to Eqs (17) - (21) for arbitrary values of a and b is the superposition $m = a \times m_a + b \times m_b$, so the full solution for the concentration profile is

$$\mu(x, t, h) = \mu_0 + (\mu_1 - \mu_0) m_a(\varepsilon, f, h) + \mu_0 \left(\frac{T_1 S_1}{T_0 S_0} - 1\right) m_b(\varepsilon, f, h) \quad (27)$$

where the x and t dependence of ε and f comes from Eq. (16).

Henry's Law invoked at the molding compound cavity interface gives the partial pressure water vapor in the cavity and Boyle's Law gives the molar concentration of water vapor in the cavity for $t > 0$ (during reflow):

$$P_{cav}(t) = \mu(x = w, t, h) / S_1 \quad (\text{Henry}) \quad (28)$$

$$\rho_{cav}(t) = P_{cav}(t) / RT_1. \quad (\text{Boyle}) \quad (29)$$

IV. EXAMPLE

The evolution of the moisture concentration given by Eqs. (27), (28), and (29) for a 0.2 cm slab of molding compound over a cavity of width 0.01 cm when subjected to a step from the preconditioning conditions to the reflow conditions of Table I is shown in Figure 2. Moisture flows into the cavity

initially increasing the cavity moisture concentration (and cavity pressure). But as drying of the molding compound propagating from the external surface approaches the cavity, the cavity concentration reaches a peak and falls away to equilibrium values corresponding to the reflow condition of Table I.

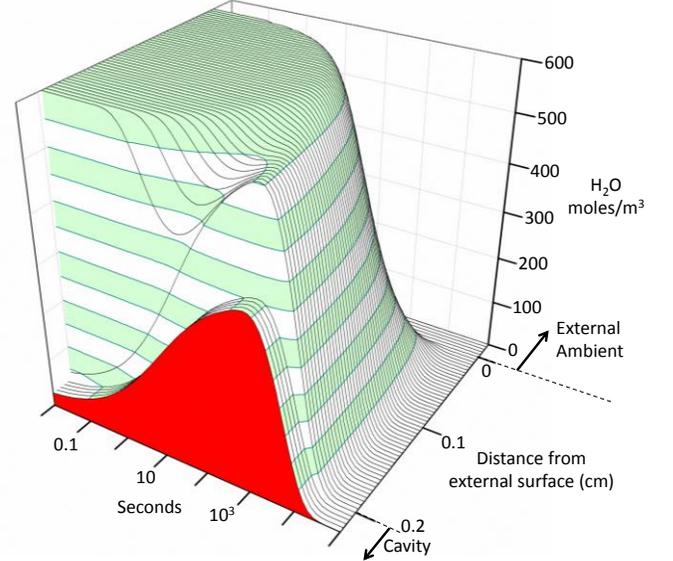


Figure 2. Evolution of molar concentration of water in a 0.2 cm slab of molding compound and a 0.01 cm cavity preconditioned and then exposed to a step reflow shown in Table I.

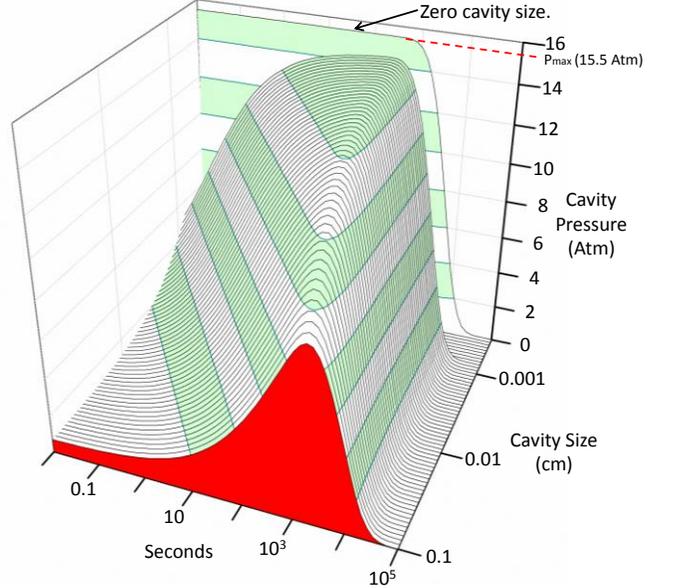


Figure 3. Evolution of cavity pressure after the step reflow of Table I for a 0.2 cm slab of molding compound for various cavity sizes. Also shown is the evolution of pressure in the limit of zero cavity size.

The evolution of cavity pressure for a slab 0.2 cm thick as a function of cavity size computed using Eq. (28) is given in Figure 3. As cavity size is reduced, the pressure rises more quickly approaching a limit, P_{max} , before falling. In the limit of zero cavity size P_{max} is reached instantly.

To derive P_{max} consider the zero cavity size limit of Eqs.

(23) and (24) as $h \rightarrow \infty$,

$$m_a(\varepsilon, f) = 1 - 2 \sum_{n=0}^{\infty} (-1)^n \gamma_n^{-1} \cos[\gamma_n(1-\varepsilon)] \exp[-\gamma_n^2 f] \quad (30)$$

$$m_b(\varepsilon, f) = 0$$

where $\gamma_n = (2n+1)\pi/2$. Eq. (30) is frequently used to compute moisture concentrations in one-dimensional models [4]. For short times ($f \ll 1$) at the cavity interface ($\varepsilon = 1$) the series sums to 1/2 so $m_a \cong 0$. From Eqs. (27), (28) and (30) the cavity pressure for zero cavity size at short times ($f \ll 1$) is,

$$P_{max} = \frac{H_0}{S_1} = H_0 P_{sat}(T_0) \frac{S_0}{S_1} = H_0 P_{sat}(T_0) \exp\left[\frac{Q_m}{R} \left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right]. \quad (31)$$

The cavity pressure may approach, but can never exceed, P_{max} . For the example of Table I P_{max} is 15.5 Atm. Eq. (31) is the same as the expression due to Bhattacharyya et al. [3]. P_{max} is independent of H_1 , is strongly dependent on T_1 , is proportional to H_0 , and is weakly dependent on T_0 . The weak dependence of P_{max} on T_0 may be seen as follows: A physically intuitive, though less accurate, Arrhenius approximation to the saturated vapor pressure may be obtained from the latent heat of vaporization, Q_{lhv} , using the Clausius-Clapeyron relation. This gives $P_{sat} = P_{\infty} \exp(-Q_{lhv}/RT)$. Using this, Eq. (31) becomes

$$P_{max} = H_0 P_{\infty} \exp\left[\frac{Q_m - Q_{lhv}}{RT_0} - \frac{Q_m}{RT_1}\right] \quad (32)$$

where $P_{\infty} = 4.58 \times 10^5$ Atm, and $Q_{lhv} = 40.7$ kJ/mole (0.42 eV). The error in the Arrhenius approximation to P_{sat} is $\pm 5\%$ between 50°C and 220°C. Eq. (32) shows the weak preconditioning temperature (T_0) dependence of P_{max} because the difference between Q_{lhv} and Q_m is only 0.02 eV. Although the dependence of P_{max} on T_0 is weak, the time to establish the level of saturation assumed by Eq. (31) is strongly dependent on T_0 since time to 90% saturation is $0.8481w^2/D(T_0)$ (about 1 year at 25°C and 230 h at 85°C for $w = 0.2$ cm).

The evolution of cavity pressure for a cavity size of 0.01 cm as a function of slab thickness for preconditioning and reflow per Table I computed using Eq. (28) is given in Figure 4. The thinner the slab, the earlier and lower is the peak pressure. As shown by the red dot in Figure 4, slabs thinner than 0.02 cm never reach the example 9 Atm threshold of damage no matter how long they are exposed to the reflow ambient, but slabs thicker than 0.02 cm reach the 9 Atm damage threshold in 13 seconds. For a cavity of 0.005 cm (not shown in Figure 4) 9 Atm is reached in 3.2 seconds for slabs thicker than 0.01 cm, but is never reached for slabs thinner than this. For zero cavity size P_{max} is reached instantaneously for any slab thickness. If P_{max} exceeds the pressure damage threshold, it may seem that limiting the time of exposure to the reflow ambient, per the IPC/JEDEC method, might be a way to prevent exposure to damaging pressures. But this depends on the existence of a sufficiently large accidental cavity to delay crossing the damage threshold and cannot be depended on. Deliberately designed-in internal cavities may be a way to use

this effect.

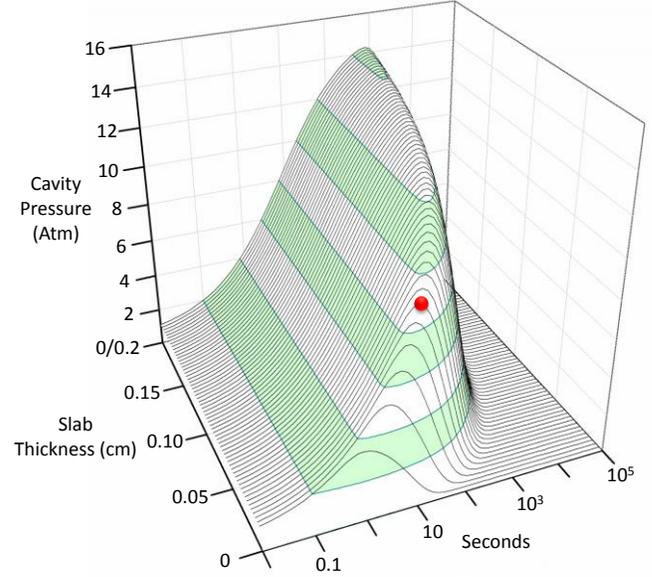


Figure 4. Evolution of cavity pressure after the step reflow of Table I for a cavity size of 0.01 cm for various slab thicknesses. The red dot shows the slab thickness (0.02 cm) which just reaches the example damage threshold of 9 Atm in 13 seconds.

V. DISCUSSION AND CONCLUSION

The boundary condition Eq. (14) relating the spatial gradient and temporal rate of change of moisture concentration at the molding compound/cavity surface gives a simple and rigorous way to account for moisture transport into and out of the cavity. The approach is an improvement on other methods of computing cavity pressure reviewed by Wong et al [5] and could be easily incorporated into more complete models which use numerical finite element methods. To model pressure in an arbitrarily shaped cavity which is not open to the ambient surrounding the package two conditions are required: 1) the moisture concentration, μ , must be constant everywhere on the cavity/molding compound interface and, 2), the following condition analogous to Eq. (14) is imposed at the cavity/molding compound interface

$$\frac{\partial \mu}{\partial t} + \frac{RT_1 S_1 D_1}{V} \oint_{\text{Cavity Surface}} \vec{\nabla} \mu \cdot d\vec{S} = 0. \quad (33)$$

In Eq. (33) V is the volume of the cavity, $\vec{\nabla} \mu$ is the moisture concentration gradient at the cavity surface, and $d\vec{S}$ is a vector element of the cavity surface normal to the surface, directed into the cavity.

For a finite cavity size Figure 3 shows that during reflow the cavity pressure rises to a peak which is more immediate and rises closer to P_{max} as the cavity size decreases. In the limit of zero cavity size the pressure reaches P_{max} instantaneously. That is, a high pressure exists at the interface of the molding compound and die or lead frame surfaces tending to separate the surfaces, *even when no cavity exists*. This pressure also exists at times and locations in the bulk of the molding compound where the molar concentration is μ_0 (the flat area on the top of the profile in Figure 2). When a

cavity does not exist the package is more robust against the popcorn effect not because the pressure “has no place to build up”, but rather as shown by Lin et al [12], because of strong adhesion between the molding compound and die or lead frame in the absence of a cavity.

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