

Vapor Pressure Prediction for Stacked-Chip Packages in Reflow by Convection-Diffusion Model

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Abstract

Moisture plays a critical role in the reliability of electronic devices, especially in the desorption process at reflow temperatures (around 270° C) when severe damages may occur due to high-pressure vapor concerted from condensed moisture. Such pressure-driven vapor flow, however, could not be described by conventional Fick's Law. Furthermore, using conventional Fick's Law for multi-materials always encounters interface discontinuity issues. Therefore, this paper adopts a Convection-Diffusion Model that is able to describe complex desorption behavior in a multi-material media without the discontinuity issue. Both pressure gradient-driven (convection) and concentration-gradient driven (diffusion) moisture transports are considered in the model. To achieve this, absorbed moisture is partitioned into vapor phase and liquid phase (condensed water), with the vapor flux governed by Darcy's Law and the water flux by Fick's Law. Henry's Law is also implemented so that the Fickian term is converted to pressure, resulting in a unified vapor pressure model. The model is applied to analyze a stacked-chip package by two numerical cases: desorption under 2 typical reflow temperature profiles. Numerical validations are also performed to show that the Convection-Diffusion Model can be reduced to traditional Fickian Model and Convection-Only Model as special cases. The numerical results show that the concentration desorption rate is much faster than that of the traditional Fickian diffusion, and somewhat faster than the Convection Model, this results in a much lower pressure in the material. However, the desorption profile with time and the pressures at low temperatures of the different models-- the Convection-Only, Diffusion-only and the Convection-Diffusion Model are indistinguishable which can be seen in both reflow profiles. The sensitivity of the CD Model to the gas permeability k and the reflow temperature profiles governs the maximum pressure that is predicted as well as the concentration content.

1. Introduction

Moisture absorption and the subsequent desorption in the semiconductor business is an important factor in the assembly of stacked-chip devices. When each part of a stacked-chip assembly is manufactured in other parts of the world, or where there is an extended storage time between production and final assembly, the opportunity for moisture intrusion is possible [1]. Thus under the soldering of the components to its final form, moisture effects

during reflow become an issue; thus failure can occur [1, 2]. The reason that failure can occur is due to the adhesive being a polymer and when heated, (without moisture) to temperatures beyond the glass transition temperature, the Young's modulus is greatly reduced, [3, 4, 5]. During the absorption phase, water vapor density is several orders of magnitude higher in the material than the surrounding air [6, 7]. Current models that use either Fick's Law or vapor pressure as the transport process, [1, 2, 3]. When the process includes large temperature ranges, the applicability of either a Diffusion Model or Convection Model is not suitable for accurate concentration prediction [2]. However, prior to the introduction of the Convection-Diffusion Model (CD Model), neither Fick's Law, nor the Sullivan and Stokes theorem (SS Model) could accurately predict the moisture loss in the material through large temperature ranges [2].

In summary of the different existing models, Fick's Law is dominant at low temperature moisture transport, but not at high temperatures [2]. The SS Model is an effective model for high temperature applications, but leaves out liquid diffusion through the media; thus there is a loss in accuracy [2]. The CD Model takes the best of both worlds and thus allows for a much more accurate moisture loss prediction [2].

This paper will show the formulation of a bi-material model of the CD Model, validation of the CD Model when reduced to either SS only model or the Diffusion-Only model, by the changing of coefficients [2]. There will be two case studies in which two thermal histories are used to predict concentration and pressure through time, and finally a sensitivity analysis of the material parameter k (vapor permeability).

2. Formulations

In order to take into account vapor flow, a Convection-Diffusion Model was proposed and validated with the experimental results by Chen and Fan, [2]. In this paper, the method will be applied to solve a multi-material problem. The general formulations of the CD Model will be introduced below.

In the CD Model, material is assumed to be porous and consists of both a solid matrix and interconnected pores. The ratio between the pore volume and the matrix volume is defined as porosity here by ϕ . Therefore, the total water density ρ_m in a porous media can be expressed as

$$\rho_m = \phi\rho_v + (1-\phi)\rho_w \quad (1)$$

in which ρ_v is the vapor density and ρ_w is the density of

concentration of water absorbed by the solid matrix (which has a volume fraction $(1-\phi)$). The volume ratio of pores, ϕ , may range from 1% to 5% for typical polymer materials, and can be determined by experimental methods, such as mercury measurement or indirect method [8, 9]. For water vapor, an ideal gas law is used convert ρ_v to pressure p :

$$\rho_v = \frac{p}{R_w T} \quad (2)$$

in which T is temperatures(K), p is pressure (pa), and R_w is gas constant for water (461.89 J/mol/K). Similarly, it would be convenient that ρ_w can also be expressed in terms of pressures. This can be achieved by using a certain isotherm according to [10]. In this paper, a modified Henry's law is used:

$$\rho_w = B \frac{p}{p_w(T)} \quad (3)$$

in which B is a constant dependent on materials and temperatures and p_w is saturated vapor pressure. Saturated pressure for water vapor (p_w) can be expressed as function of temperature:

$$p_w = p_{w0} \exp(A_3/T) \quad (4)$$

in which p_{w0} is 36839.4 MPa and A_3 is -4802.4 K [11].

In the CD model, the total moisture flux includes both vapor flux and water flux, and their driven mechanism are fundamentally different. For water vapor, its driving force is pressure and its flux $J(\rho_v)$ can be described by a widely-used Darcy's law, as

$$J(\rho_v) = \frac{\rho_v k}{\mu(T)} \nabla p = \frac{pk}{R_w T \mu(T)} \nabla p \quad (5)$$

in which k is permeability, μ vapor viscosity dependent on temperature. Permeability k is a material property and could be a function of porosity [12] and does not change with temperatures. Viscosity of water vapor can be determined by temperatures according to CRC handbook [13], as

$$\mu(T) = 1.0075e^{-6} \sqrt{\frac{T}{647.27}} \left(0.0181583 + \frac{0.0177624}{T} + \frac{0.0105287}{\left(\frac{T}{647.27}\right)^2} - \frac{0.0036744}{\left(\frac{T}{647.27}\right)^3} \right) \quad (6)$$

For the water in the solid matrix, its driving force is concentration gradients and can be described by the conventional Fick's law, which state that:

$$J(\rho_w) = D(t) \nabla \rho_w \quad (7)$$

in which $D(T)$ is diffusion coefficient dependent on temperature.

Once the vapor flux and water flux are calculated, we can apply the law of conservation of mass for moisture changes in porous media with time, as:

$$\phi \frac{\partial \rho_v}{\partial t} + (1-\phi) \frac{\partial \rho_w}{\partial t} = \nabla \cdot [J(\rho_w) + J(\rho_v)] \quad (8)$$

in which both diffusion of concentrated water and convection of water vapor are considered. By substituting (2), (3), (5), and (7) into (8), we obtain a convection-diffusion model as:

$$\frac{\phi}{R_w} \frac{\partial(p/T)}{\partial t} + (1-\phi) B \frac{\partial(p/p_w)}{\partial t} = \frac{k}{\mu RT} \nabla \cdot (p \nabla p) + \frac{BD}{p_w} \nabla^2 p \quad (9)$$

in which the first term on the right-handed side represents a convective flow, while the second term represents a diffusive flow. The convection-diffusion equation assumes a uniform heating case (e.g. Temperature does not vary within the material).

Since the diffusion-convection equation in (9) solves vapor pressures directly, initial and boundary conditions in terms of vapor pressures need to be defined. If initial temperature T_0 and relative humidity $R.H.$ are known, the initial vapor pressures will be given as:

$$p_{int} = p_w(T_0) R.H. \quad (10)$$

Similarly, if the ambient temperature T_{ab} and $R.H._{ab}$ are known, then the vapor pressure at the boundary becomes

$$p_{bc} = p_w(T_{ab}) R.H._{ab} \quad (11)$$

When there is no moisture transport across a barrier, such as between silicon and the adhesive, a Neumann boundary condition is used, in which mathematically is zero flux

$$\frac{dp}{dx} = 0 \quad (13)$$

As stated by Chen and Fan [2], CD model may be reduced to traditional Fickian model or convection-only model (SS model), [2]. When vapor permeability and porosity is neglected, Eq. (9) will be similar to Fickian model; when water diffusivity $D(T)=0$, Eq.(8) will be similar to SS model.

3. Numerical Validation

To verify the CD Model, each component must be evaluated to meet current experimental and theoretical results. The solution of the model is implemented in MATLAB and uses the MATLAB's function ODE15s for the time step. The space step uses the central difference scheme in which the coefficients are both functions of space and of time/temperature.

3.1 Validation of CD Model with SS Model

To verify the SS Model, the CD Model must be used with the corresponding Fick's Law components equaling zero. Thus, the CD Model returns to the SS model, as:

$$\left\{ \frac{\phi}{R_w T} + (1-\phi) \frac{B}{p_w} \right\} \frac{\partial p}{\partial t} - \frac{k}{\mu R_w T} \frac{dp}{dx} \left(p \frac{dp}{dx} \right) = \left[\frac{\phi}{R_w T^2} + \frac{(1-\phi)}{p_w^2} \frac{dp_w}{dT} \right] T p \quad (14)$$

Validation data of the SS model is from the work by Muralidharan's et.al. [11] and these results are what are used to validate the CD Model. In table 1 the parameters are shown for the validation and case studies.

Table 1. Material Properties for Validation Cases.

Parameter	SS [11]	Only	Diff. Only
$L(\text{mm})$	1		0.2
ϕ	10%		0%
$R.H.$	100%		100%
$B(\text{Kg/m}^3)$	54		6
$k(\text{m}^2)$	$2.7\text{e-}20$		0
A	0		9.5
$\tilde{T}(\text{K})$	/		300
$D_0(\frac{\text{m}^2}{\text{s}})$	0		$2.14\text{e-}12$

The material is 1 mm in length and has Dirichlet boundary conditions at both ends, which can be seen in Figure 1. The Initial vapor pressure is based on steam tables, with a function approximating the steam table values and can be seen in equation (5). The heating profile is a ramp profile, which can be seen in Figure 2.

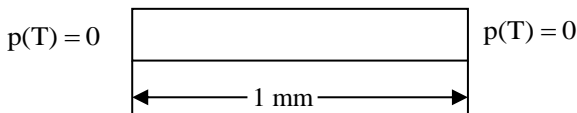


Figure 1. Geometric Layout and Boundary Conditions for Convection-Only CD Model Verification.

Using the profile in Figure 2 and the corresponding properties, the validation of the SS model in the form of the CD Model is verified. The results of the CD Model verification can be seen in figure 3. The validation is complete for the CD Model; there are some very small differences, but that is due to the solver that they used--they used ODE23s, and this paper uses ODE15s, which computes the time step completely differently. Thus with such small differences the code is verified [11].

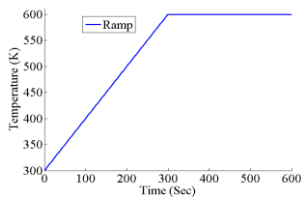


Figure 2. Thermal History for Rapid Heating.

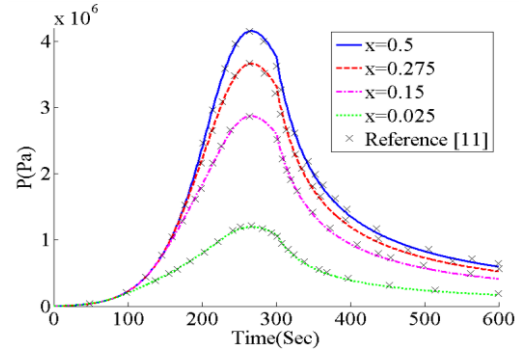


Figure 3. CD Model Validation Compared to SS Model [11].

3.2 Validation of CD Model with Diffusion-only Model

With vapor permeability equal to zero, a diffusion-only model can be found:

$$\frac{dp}{dt} = D(T) \nabla^2 p \quad (15)$$

where $D(T)$ follows the Arrhenius equation :

$$D(T) = D_0 \exp\left(A\left(1 - \frac{\tilde{T}}{T}\right)\right) \quad (16)$$

in which constant A is a material constant, D_0 is the diffusion coefficient at reference temperature \tilde{T} [14].

Next shown is the validation of the Diffusion model which is seen in equation (16). The validation of this part is compared to the results that ANSYS gives for the following material properties and geometries, and the set up can be seen in Figure 4. It has a Dirichlet boundary condition on one side and a Neumann boundary condition on the other.

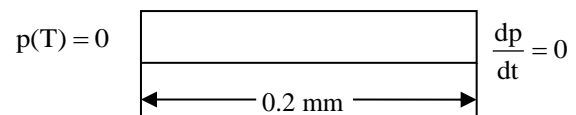


Figure 4. Geometric Layout and Boundary Conditions for Diffusion-Only CD Model Verification.

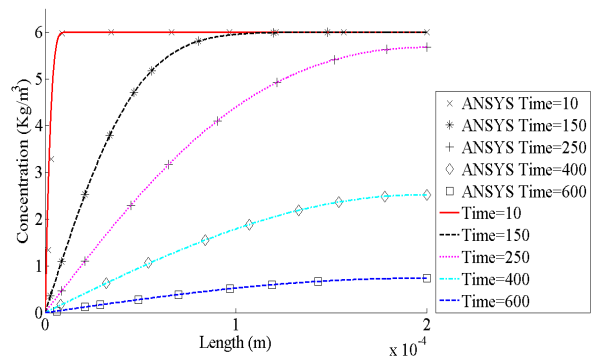


Figure 5. Diffusion-only Verification of CD Model with FEM.

Using this setup, the diffusion validation is based on the concentration profiles through the 0.2 mm length and evaluated at times of 10 seconds, 150 seconds, 250 seconds, 400 Seconds, and 600 Seconds. As can be seen in Figure 5, the CD Model with the SS coefficients set to zero match quite closely.

4. Numerical Applications

4.1 Problem Statement

The analysis of stacked-chips can be simplified from a 3D case to a 1D model because of symmetry. The 3D case first is thought of as a 2D slice of the material as can be seen in Figure 6.

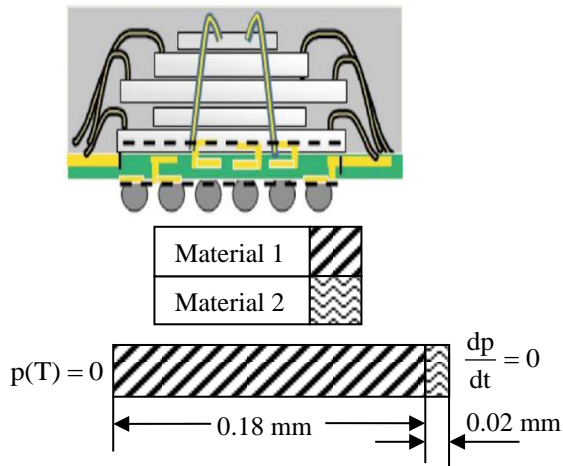


Figure 6. Stacked-Chip layout and 1D simplification for CD Model Case Studies.

The CD Model is derived as a 1D model and can be thought of a slice of a 2D model. Since the moisture does not get in the adhesive layers between the silicon chips, the only the substrate and the subsequent thin film adhesive will be looked at, [1, 3]. As in Figure 7 the model ignores the silicon itself by using a zero flux term at the edge where the thin film meets the silicon, this allows for the concentration to be non-zero. The other layers of thin film are not looked at because the major failure location is between the substrate and the thin film [1, 2, 3]. The reflow case study is meant to show the dependency of maximum pressure and concentration desorption rate based on both temperature reflow profiles, and the sensitivity of permeability on the overall pressure. Another objective of the two different reflow profiles is to emphasize the difference between the Convection-Only Model (SS model) and Diffusion-Only Model (Fick's Law), when compared to the CD Model.

With that being said, the preliminary initial conditions and boundary conditions are as follows. The geometric layout can be seen in Figure 6. The boundary conditions for all models, except the sensitivity analysis, use the same material properties and boundary conditions. The initial temperature, and

thus the initial pressure, will be different, since the initial vapor pressure is determined by the initial. The values of $D(T)$ are a function of time and follow an Arrhenius equation that takes the value of D_0 at a certain temperature. The value of $D(T)$ is exponential and thus is highly sensitive to temperature; this will be an important factor when analyzing the results of the two different reflow profiles. With these coefficients, a comparison between the two temperature loading profiles shown in Figure 7 is done. The saturated vapor pressure can be estimated using the function from in equation (5), [11].

Table 2. Material properties for CD Model Case Studies

Parameter	CD Model	
	Mat_1	Mat_2
$L(\text{mm})$	0.18	0.02
ϕ [3, 15, 16]	5%	5%
$R.H.$	60%	60%
$B(\text{Kg}/\text{m}^3)$	6	4.512
$k(\text{m}^2)$	1e-20	1e-20
A	9.5	9.56
$\bar{T}(\text{K})$	272	275
$D_0(\frac{\text{m}^2}{\text{s}})$	2.14e-12	2.93e-11

The reflow profiles in Figure 7 are derived from real reflow profiles and curve fitted with an 8 term sum of sin equation that fits the original data with an R^2 of 0.998 for both curves, [3, 4]. This was done so that the equation for temperature can be shown as a function of time and its derivative as well. This gives a smooth result and makes it easy to compare results.

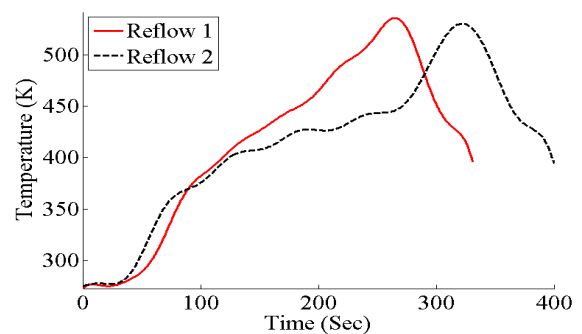


Figure 7. Temperature Loading Profiles [3, 4].

4.2 Results Based on Reflow 1

In Figure 8, the results show concentration at the edge of the material, where the adhesive meets the silicon; this is the area that fails when failure occurs [3]. Since this is the area of interest, all pressure, and

concentration with respect to time graphs will be evaluated at this location.

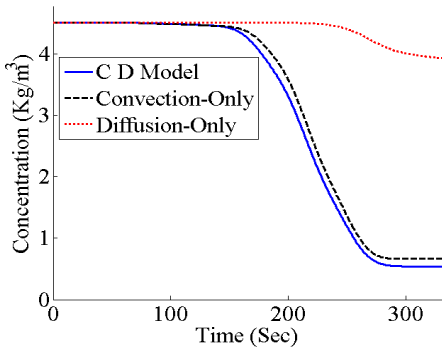


Figure 8. Moisture Concentration at Adhesive Silicon Interface Vs Time (Reflow Profile 1).

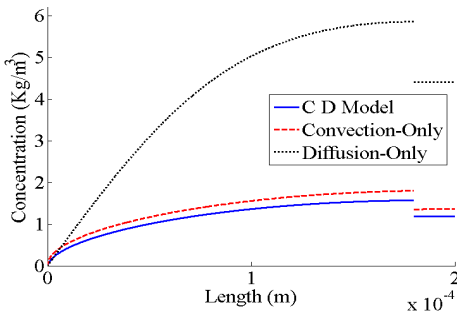


Figure 9. Concentration Contours at 250 seconds (Reflow Profile 1).

From equation (9) the CD Model can be seen as nonlinear. From Figures 8 and 10 the nonlinearity can be seen in that the principle of superposition does not work, where no two models sum to equal the third model. This is due to the individual natures of the SS and Fickian models which are coupled together through pressure. At low temperature the driving pressure is from diffusion and the SS pressure contribution is small, but as the temperature rises, the vapor flow from the SS model becomes significant. Thus there is a transition from diffusion driven, to vapor flow driven mass transfer. It is seen in Figure 8 that the rate of desorption based on the concentration of the material at the edge interface between the silicon and thin film is much slower for the diffusion-only model, when compared to the convection-only (SS model) or the CD Model. This means that there is still a lot of liquid in the material when the temperature is at the greatest point, thus there is over a magnitude in order difference in the level of pressure between the CD Model and the diffusion model as can be seen in Figure 10. Figure 8 shows that if the diffusion is the only model used, then the estimated water content will

be drastically over-estimated. It also this shows that for the first 150 seconds the models are basically the same and there is no significant difference. This means that the CD model and the SS model have no distinct advantage at low temperatures; only when there are high temperatures with large temperature ranges is there a significant difference.

Concentration versus the length of the specimen is looked at next. The moisture content of the material can be determined, and as in Figure 9, it clearly shows that the moisture content at 250 seconds is much greater than either the SS Model or the CD Model. Shown in Figure 10 are the vapor pressure results for the CD Model, Fick's Law and SS model for reflow profile 1.

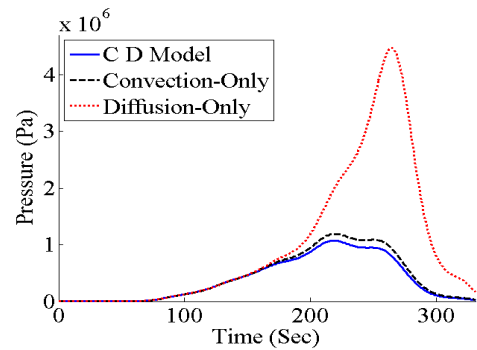


Figure 10. Vapor Pressure at Adhesive Silicon Interface.

4.4 Results Based on Reflow 2

The second reflow profile is evaluated and the results are similar to the ones in Reflow 1, but the pressure of the Diffusion-Only Model is a little less than the Reflow 1 profile and the maximum pressure is offset to a later time. This follows the Reflow 2 temperature profile where it takes longer to reach the maximum temperature. The concentrations of the different models are also similar to Reflow 1, and thus the amount of water left in the material is similar. As can be seen in Figure 11, the moisture content looks very similar each other in the manner of desorption, but rather an offset of the amount of water at any given time after 200 seconds.

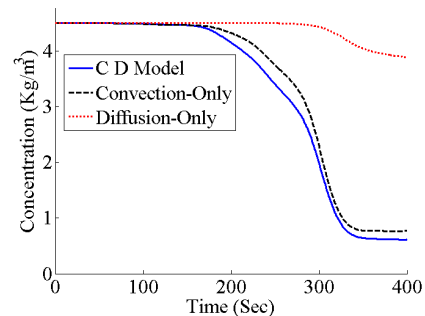


Figure 11. Concentration at Adhesive Silicon Interface Vs Time (Reflow 2).

This is shown in the concentration contours in Figure 12, when the concentration is observed at 250 seconds and the difference is an offset and not drastically different. It even shows that the SS model over-estimates the amount of water still in the material, which is important to note because there cannot be any firm conclusion made from the concentration, because it is highly dependent on the temperature profile and the rate at which the temperature rises.

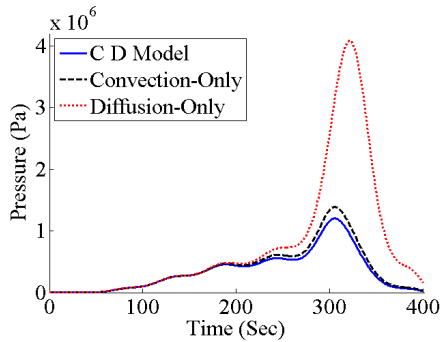


Figure 12. Concentration Contour (Reflow 2).

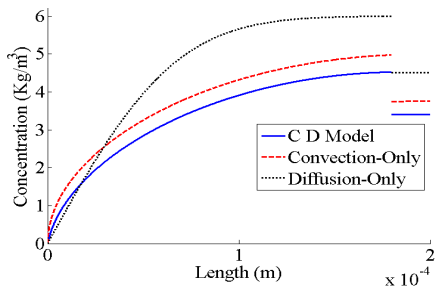


Figure 13. Reflow 2 Pressure at Adhesive Silicon Interface (Reflow 2).

4.5 Comparison of CD Model: Reflow 1 vs. Reflow 2

So far the discussion has been about the differences among the Diffusion-Only, Convection-Only (SS) and the CD Models-- but now it is important to take a closer look at the CD Models' response to the different temperature profiles and to see the dependency of the model on the material property permeability. The first section deals with the comparison of the two reflow profiles. In Figure 16 the pressures of both reflow profiles are shown. The pressure of reflow profile 2 is higher than that of reflow profile 1 when the CD Models are compared.

However, the concentration with respect to time, Figure 14, shows that the amount of liquid is higher in the material during reflow 2 than that of reflow 1. This makes sense, because the temperatures at any given time are drastically different. This means that concentration is not directly related to the current pressure, the saturated vapor pressure must also be taken into account which also is an Arrhenius equation,

[11]. This means that the relationship between saturated vapor pressure equation (4) and concentration depends on two different exponential equations-- one for the diffusion coefficient and the other for the saturated vapor pressure.

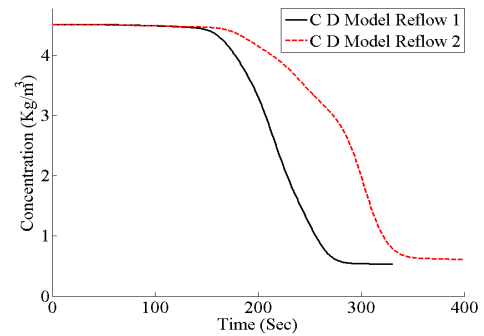


Figure 14. CD Model Concentration at adhesive silicon interface vs. Time.

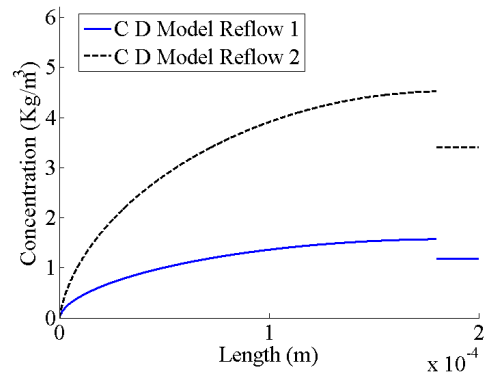


Figure 15. Concentration Contours.

When the concentration contours are observed, Figure 15, the results are as now expected: the reflow profile 1 has less moisture, and reflow profile 2 has more. This is because the temperature of each material is at during the reflow process-- the temperature of reflow 2 at 250 seconds is about 100° C less than that of Reflow 1. Thus, at 250 seconds there is a large difference in the concentration. But as can be seen in Figure 14, the concentration eventually reaches the same level as Reflow 1; it just takes longer.

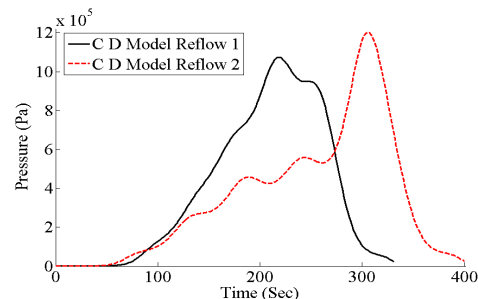


Figure 16. CD Model Pressure at Adhesive Silicon Interface: Reflow 1 and 2.

The CD Model should approach the diffusion model when the permeability goes to zero. To illustrate this, a sensitivity analysis is done. As can be seen in Figure 18, as the permeability decreases, the pressure sharply increases, for both reflow profile 1 and for reflow Profile-2.

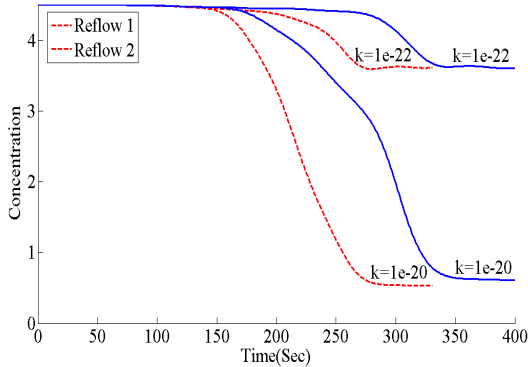


Figure 17. Concentration at Adhesive Silicon Interface vs Time—Sensitivity of CD Model to permeability k .

It can be seen that the lower the gas permeability goes the higher the pressure goes. This is to be expected and will continue to increase until it reaches the final diffusion-only term. However, there is an increase in the time taken to reach the final pressure, so the whole process will take longer, and eventually will not be distinguishable from the diffusion terms. Also the concentration when plotted versus time the effect of reducing permeability can be easily seen. As in Figure 17, the concentration rates drop as the permeability gets smaller.

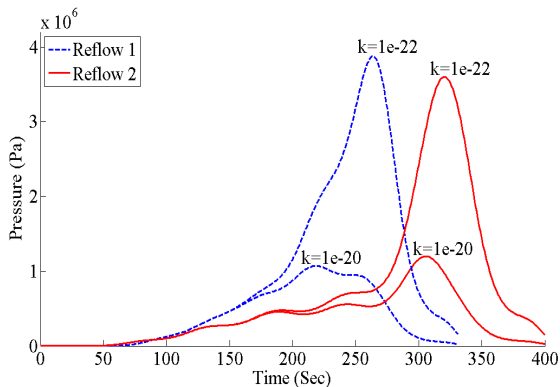


Figure 18. Pressure sensitivity of CD Model with k , at Adhesive Silicon Interface.

The reflow 2 profile, difference can be described in the heating rate is different so the pressure follows another saturated vapor curve than reflow 1. The effects of permeability are not completely clear because there is a large dependence on the temperature profile rather than just material properties. Because of this, the results of the sensitivity analysis only show

that a decrease in permeability will drive the concentration to the diffusion-only values. This does not, by itself, describe the sensitivity of the rate of moisture loss, thus the temperature reflow profiles and the saturated vapor pressures must be considered as well.

5. Conclusions

In conclusion it is seen that the overall description of the CD Model predicts much lower pressures in the material which is highly dependent on the material property: vapor permeability k and the temperature loading histories, the reflow profiles. But k is not enough to describe the behavior of the systems reaction, but the temperature profile and heating rate must be considered as just as important as the material properties. This is due to the concentration being derived from the pressure of the system in which both vapor flow convection and Fickian diffusion contribute to the pressure. The coefficients of both saturated vapor pressure and the diffusion coefficient change with time in an exponential manner, thus the results are highly sensitive to the temperature and the concentration reflects this. This result is expected since, restricting the permeability of the material would force the diffusion to transport the moisture. Thus we see the large spike in pressure. The concentration when looked at with respect to time, the rate at which it is desorbs is much greater for the CD Model rather than the Diffusion model, this is also expected in that when only diffusion is taken into account, the lower the permeability the more time it takes for the diffusion part to supplement the corresponding loss in vapor flow. Thus the CD Model predicts desorption in a much more conservative way and is highly dependent on the permeability of the material and temperature reflow profiles.

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