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A Review on Water Vapor Pressure Model for Moisture Permeable Materials Subjected to Rapid Heating

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ABSTRACT

This paper presents a comprehensive review and comparison of different theories and models for water vapor pressure under rapid heating in moisture permeable materials, such as polymers or polymer composites. Numerous studies have been conducted, predominately in microelectronics packaging community, to obtain the understanding of vapor pressure evolution during soldering reflow for encapsulated moisture. Henry's law based models are introduced first. We have shown that various models can be unified to a general form of solution. Two key parameters are identified for determining vapor pressure: the initial relative humidity and the net heat of solution. For materials with nonlinear sorption isotherm, the analytical solutions for maximum *vapor pressure are presented. The predicted vapor pressure, using either linear sorption isotherm (Henry's law) or nonlinear sorption isotherm, can be greater than the saturated water vapor pressure. Such an "unphysical" pressure solution needs to be further studied. The predicted maximum vapor pressure is proportional to the initial relative humidity, implying the history dependence. Furthermore, a micromechanics-based vapor pressure model is introduced, in which the vapor pressure depends on the state of moisture in voids. It is found that the maximum vapor pressure stays at the saturated vapor pressure provided that the moisture is in the mixed liquid/vapor phase in voids. And, the vapor pressure depends only on the current state of moisture condition. These results are contradictory to the model predictions with sorption isotherm theories. The capillary effects are taken into consideration for the vapor pressure model using micromechanics approach.*

Keywords: moisture permeable, moisture diffusion, rapid heating, Henry's law, nonlinear sorption isotherm, micromechanics, soldering reflow, electronic packaging

Nomenclatures

C	Moisture concentration, kg/m^3
C_{sat}	Saturated moisture concentration, kg/m^3
P_{amb}, P_{sat}	Ambient vapor pressure and saturated water vapor pressure, Pa
S	Henry solution coefficient, kg/m^3/Pa
S_∞	Prefactor to calculate S, kg/m^3/Pa
ΔH_s	Heat of solution to calculate S, J/mol
R	Universal gas constant, 8.314 J/mol/K
T	Temperature, K
k_H	Henry's constant, $k_H=1/(SP_{sat})$, m^3/kg
RH_{amb}	Ambient relative humidity
C_{cav} ,ρ_{cav}	Moisture concentration and density at cavity surface, respectively, kg/m^3
P_{cav} , P_{max}	Cavity pressure and its maximum pressure during heating, Pa
w, l	Thickness and cavity size, respectively, m

D	Moisture diffusivity coefficient, m^2/s
D_1	Diffusion coefficient at T_1, m^2/s
D_∞, E_D	Prefactor (m^2/s) and activity energy (J/mol), respectively, for calculating D
C_0, C_1	Initial and boundary moisture concentration for preconditioning and reflow, respectively, kg/m^3
T_0, T_1	Preconditioning and reflow temperature, respectively, K
RH_0, RH_1	Initial and reflow relative humidity, respectively, $RH= P_{amb} / P_{sat}$
P_{sat0}, P_{sat1}	Saturated water vapor pressure at T_0 and T_1, respectively, Pa
P_0	Ambient water vapor pressure for preconditioning, Pa
R_w	Water gas constant, 461.6 J//kg/K
$\bar{x}$, $\bar{t}$	Normalized position and time for Shirley's solution
h	Normalized parameter in Shirley's solution
P_∞	Prefactor in Clausius–Clapeyron relation for P_{sat}, Pa
ΔH_{vap}	Heat of vaporization for water, J/mol
g, X, τ	Normalized concentration, position, and time for Hui's solution
α	Normalized parameter in Hui's and Chen's solution
ΔH_s^*	Net heat of solution, $\Delta H_s^* = \Delta H_s - \Delta H_{vap}$, J/mol
k_∞	Prefactor for calculating k_H, $k_\infty = 1/(p_\infty S_\infty)$, m^3/kg
W_d	Dynamic wetness at cavity surface, $W_d = C_{cav}/C_{sat}$
ϕ, ϕ_{eq}	Porosity and equivalent porosity, respectively
$\dot{T}$	Heating rate, K/s
K_H	Henry solubility constant (=$1/k_H$ when ΔH_s^*=0 kJ/mol)), kg/m^3
P_v	Water vapor pressure in free volumes or pores, Pa
κ, μ	Vapor permeability (m^2) and viscosity (Pa·S), respectively
a_w , $a_{w,eq}$	Water activity and equilibrium ambient water activity, respectively
f_C , f_a	Water sorption isotherm functions, $f_C = C(a_w,T)$; $f_a = a_w (C, T) = f^{-1}_C$
Q_{st}	Isosteric heat of water sorption, kJ/mol
Q^*_{st}	Net isosteric heat of water sorption, $Q^*_{st} = Q_{st} - \Delta H_{vap}$, kJ/mol
$\mathbf{J}$	Water flux, $kg/m^2/s$
B	Mobility of water molecules, $mol \times m^2/s/J$
μ_w, μ_{w0}	Water chemical potential and its reference value, J/mol

K	Generalized solubility which is a function of T and a_w, kg/m^3
ρ_a, ρ_g	Apparent and saturated moisture density, kg/m^3
A	Cavity surface, m^2
M	Mass of water vapor in cavity, kg
V	Cavity volume, m^3
G_1	Empirical constant for Sawada’s model, Pa·m^3/kg/K
V_m	Molar volume of water, $=1.8\times10^5$ m^3/mol
P'_{sat}	Modified saturated vapor pressure in microvoids, Pa
ρ'_g	Modified saturated vapor density, kg/m^3
$\sigma(T)$, σ_{rm}	Water surface tension at T and room temperature, respectively, N/m
r	Radius of microvoids, nm
θ	Water contact angle of microvoids, degree

1. INTRODUCTION

Polymers or polymer composites play a significant role in the advancement of technology in microelectronics, deformable electronics, and microelectromechanical system (MEMS) [1, 2]. However, most polymers and their composites are inevitable to moisture absorption, which will alter physical properties and greatly compromise material performance [3-6], such as diminished glass transition temperature T_g [7], volumetric swelling [8-11], loss in modulus and strength [12-15], and interfacial adhesion degradation [16-21]. Moreover, the “encapsulated” moisture in material may cause popcorn blistering failure subjected to the increasingly hostile environment, for example, to a higher reflow temperature with the new lead-free solders and nanoparticle sintering process [22-28]. Water vapor pressure grows exponentially with temperature and thus becomes substantially high at a temperature as high as 300 ^{o}C. Extremely high steam pressure is generated due to the phase change of the encapsulated moisture at elevated temperature. As an extreme case, the softened material is further damaged by water vapor when a macroscopic crack develops and propagates to the exterior. An audible sound will be produced with a sudden release of water vapor. This phenomenon is the so-called popcorn failures and well observed in plastic integrated circuit (IC) packages [16, 17, 23-26, 28].

Figure 1 shows an example of polymer adhesive film rupture in a stacked-chip microelectronic package during reflow soldering process after moisture absorption, which followed an industrial standardized moisture sensitivity test [28]. Massive cohesive film ruptures were observed at the bottom layer of polymeric thin films that are used for chip bonding to the substrate (Fig. 1a). Fig. 1b reveals the details of the damage of film from a top-down microscopic view of the film.

Vapor pressure-induced failures were also reported for graphite/polyimide laminates used in aerospace applications [29, 30]. As shown in Fig. 2, both dry and moisture-saturated specimens were tested under thermal spikes from room temperature to 310 °C. The recorded strain-temperature data (Fig. 2a) indicate that moisture-saturated specimens experienced much larger deformation during the process in comparison to the dry ones, with an abrupt increase of strain occurring at 300 ^{o}C. The microscopy in Fig. 2b shows that many spherical microvoids were generated by high water vapor pressure, which grew and filled the entire mid-plane layers of the laminate at 310 ^{o}C.

Encapsulated moisture is a unique form of mechanical load, which evolves and is coupled with moisture diffusion, water vapor flow, phase change, heat transfer, and more significantly, material’s microscopic degradation [31, 32]. Over the last two decades, numerous studies have been made, predominately in microelectronics packaging community, to gain the fundamental understanding associated with moisture absorption and vapor pressure evolution [17, 33-40]. One of the poineering works in [25] treated the moisture diffusion by heat condution equations. Then, stresses induced by moisture and temperature are modeled in the combined form for a packaging structure subjected to encapsulation and reflow soldering. Interface gaps are explicitly modeled by rigirous contact mechanics and interfacial mechanics. Time dependent vapor pressure is also modeled. Yet, vapor pressure induced failures still persist with today’s new product development in 3D IC technology. Many new materials, such as super-hydrophobic coating, are effective in protecting device/component from water attack, but they have shown negligible resistance to ambient humidity environment, and thus no resistance to blistering failure during rapid heating [5, 41].

Vapor pressure evolution during rapid heating is presumed to be a dominant driving force for failure. Different theories and models have been developed to characterize vapor pressure in relation with moisture diffusion and microscopic feature. However, a variety of formulations for vapor pressure yield different results, and no consensus has been reached on the assumption and results obtained in each model. The aim of this paper is to provide a comprehensive review and comparison of different theories and models for water vapor pressure in moisture permeable material. We recognize that the existing theories can be grouped into two categories: Henry's law-based and micromechanics-based models. For the former, by assuming an existence of a "macro cavity" in material, or introducing porosity, several theories and models using different assumptions and approaches are present in the literature [34-36, 42, 43], which give different results. This paper reexamines the exisiting theoretical solutions based on a generalized Henry's law approach. The models that consider the effect of the dynamics of vapor flow are also discussed [37, 44, 45]. Furthermore, the generalized frameworks to consider non-Henry sorption isotherms for vapor pressure prediction are developed in this paper.

Different from Henry' law-based vapor pressure models, micromechanics-based model assumes that moisture resides in micro-/nano-sized pores or voids, which are responsible for vapor pressure development. This paper will review the two-phase micromechanics-based vapor pressure model [38-40] and the semi-infinite media pressure model [46], and the results are compared to Henry's law-based models. The paper further develops a modified micromechanics based model to consider the capillary effect that could significantly lower the calculated water vapor pressure.

The paper is organized as follows. In Sec. 2, various analytical solutions based on Henry's law, using 1-D problem, are presented and compared. A unified formulation is developed, with which the history effect of initial relative humidity and the presence of unphysical pressure are discussed. Section 3 reviews two porous media models that consider water vapor flow in water vapor pressure analysis. Section 4 proposes two generalized frameworks to consider non-Henry moisture sorption isotherms. Section 5 reviews and compares micromechanics-based models against the isotherm-based models. A modified model is developed in Sec. 6 to consider the capillary effect on water vapor pressure in microvoids. Concluding remarks are drawn at the end.

2. HENRY'S LAW-BASED MODELS

2.1 Shirley's Solution

Consider a moisture permeable material in equilibrium with a humid ambient with ambient vapor pressure, P_{amb}. Henry's law establishes a relationship between the ambient vapor pressure and the moisture concentration in solid matrix, as follows [47-49]

$$C_{sat}(T) = S(T)P_{amb} = S_{\infty}\exp\left[\Delta H_s/(RT)\right]\cdot P_{amb} \tag{1}$$

where C_{sat} is the saturated moisture content in the solid, S is Henry solubility that is dependent on temperature T, S_{∞} is a pre-factor, ΔH_s is the heat of solution, and R is universal gas constant.

Henry's law in Eq. (1) can also be written as

$$C_{sat} = S(T)P_{sat}\frac{P_{amb}}{P_{sat}} = \frac{RH_{amb}}{k_H} \tag{2}$$

where P_{sat} is saturated water vapor pressure, $k_H = \left(SP_{sat}\right)^{-1}$ called Henry constant, and RH_{amb} is ambient relative humidity.

To apply Henry's law for water vapor pressure analysis, a cavity is typically assumed at the place of interest in material, thus,

$$P_{cav}(t) = C_{cav}(t)/S(T) = k_H P_{sat} C_{cav}(t) \tag{3}$$

where P_{cav} is cavity pressure and C_{cav} is the moisture concentration at cavity surface.

Shirley [35] conducted an analytical study on a 1-D cavity pressure problem as depicted in Fig. 3. The 1-D problem represents a typical and simplified microelectronic assembly of an epoxy molding compound and lead frame. The compound can absorb a significant amount of moisture, while the lead frame (made of copper in most of the applications) is water-impermeable. Between the compound and the lead frame, there is a cavity to represent a crack or void along the interface. The system is initially in equilibrium with the preconditioning ambient with RH_0 and T_0, and then subjected to a reflow soldering process simulated by a step change from T_0 to the reflow temperature T_1. The ambient humidity is also changed to RH_1 ($<RH_0$) to represent a drying process. To analyze this problem, two main assumptions are made in [35]: 1) the material and cavity are rigid, and 2) the heating is uniform across the whole model.

To describe moisture diffusion, the Fick's second law was used:

$$\partial C(x,t)/\partial t = D_1 \partial^2 C(x,t)/\partial x^2, \quad 0 < x < w \tag{4}$$

where C is moisture concentration at location x and time t, $D_1 = D(T_1)$ is diffusion coefficient at reflow temperature T_1, and w is thickness. Water diffusivity is often described by Arrhenius equation as $D(T) = D_\infty \exp\left(-E_D/RT\right)$, where D_∞ is a pre-factor and E_D is activity energy [35, 36].

The initial condition is written as

$$C(x,t=0) = C_0 = S_0 P_{sat0} RH_0, \quad 0 < x < w \tag{5}$$

where $S_0=S(T_0)$ and P_{sat0} is P_{sat} at T_0. The boundary condition at material surface x=0 is

$$C(x=0,t) = C_1 = S_1 P_{sat1} RH_1, \quad t > 0 \tag{6}$$

where $S_1=S(T_1)$ and P_{sat1} is P_{sat} at T_1.

At cavity surface x=w, the step change of temperature at t=0 leads to a jump in cavity pressure according to Boyle's law, as P_{cav} (t=0+) =P_0T_1/T_0 (P_0 is the initial cavity pressure). Thus, there is sudden change in moisture concentration at the cavity interface x=w:

$$C(x = w, t = 0+) = S_1 P_{cav}(t = 0+) = S_1 P_{sat0} RH_0 T_1 / T_0 \tag{7}$$

which serves as one boundary condition. In addition, the mass of moisture must be balanced at the cavity interface, as

$$-D_1 \frac{\partial C}{\partial x}\bigg|_{x=w} = l \frac{\partial \rho_{cav}}{\partial t} \qquad \text{or} \qquad \frac{\partial C}{\partial x} + \frac{l}{D_1 R_w T_1 S_1} \frac{\partial C}{\partial t}\bigg|_{x=w} = 0 \tag{8}$$

where l is cavity width, R_w is gas constant for water molecules, and water vapor density $\rho_{cav} = P_{cav} / (R_w T) = C_{cav} / (R_w T S_1)$ based on the ideal gas law and Henry's law.

Equations (4)~(8) can be solved by the superposition of the existing solutions in VanSant's report [50], resulting in the Shirley's solution for moisture concentration, as [35]

$$C^{Shirley}(\bar{x}, \bar{t}, h) = C_0 + (C_1 - C_0) m_a(\bar{x}, \bar{t}, h) + C_0 \left(\frac{T_1 S_1}{T_0 S_0} - 1 \right) m_b(\bar{x}, \bar{t}, h) \tag{9}$$

with

$$m_a(\bar{x}, \bar{t}, h) = 1 - \sum_{n=1}^{\infty} \frac{2(\gamma_n^2 + h^2)}{\gamma_n (\gamma_n^2 + h^2 + h)} \sin(\gamma_n \bar{x}) \exp(-\gamma_n^2 \bar{t});$$

$$m_b(\bar{x}, \bar{t}, h) = \sum_{n=1}^{\infty} \frac{2h}{(\gamma_n^2 + h^2 + h)} \frac{\sin(\gamma_n \bar{x})}{\sin(\gamma_n)} \exp(-\gamma_n^2 \bar{t})$$

where $\bar{x} = x / w$, $\bar{t} = D(T_1) t / w^2$, $h = R_w T_1 S_1 w / l$, and γ_n is the positive roots of $\gamma_n \tan(\gamma_n) = h$.

Cavity pressure is then evaluated by substituting $C^{Shirley}(1.0, \bar{t}, h)$ into Eq. (3) or Henry's law, as:

$$P_{cav}^{Shirley} = C_{cav}^{Shirley} / S_1 = C^{Shirley}(1.0, \bar{t}, h) / S_1 \tag{10}$$

which is the Shirley's solution to cavity pressure.

For demonstration, the calculated cavity pressure is plotted in Fig. 4 for different values of *h* with the material properties given in [35]. In general, cavity pressure becomes higher as *h* increases (a larger *h* means a greater ratio between the material thickness and cavity size). There exists a maximum pressure $P_{\max}$ ($<P_{sat1}$) for the case of $h \rightarrow \infty$, which occurs when the cavity size approaches zero. The "zero-size" cavity solution was found by taking the limit of Eq. (9) with $h \rightarrow \infty$, as [35]

$$C_{cav\to 0}^{Shirley}(\bar{x},\bar{t};h\to\infty)=C_0+(C_1-C_0)\left(1-2\sum_{n=0}^{\infty}(-1)^n\gamma_n^{-1}\cos[\gamma_n(1-\bar{x})]\exp(-\gamma_n^2\bar{t})\right) \tag{11}$$

where $\gamma_n=(2n+1)\pi/2$ and $P_{cav\to 0}^{Shirley}=C_{cav\to 0}^{Shirley}/S_1$. Shirley [35][35] showed that the zero-cavity solution in Eq. (11) resembles the widely-used solution of 1-D diffusion models where no moisture transfer at cavity surface was considered.

The maximum vapor pressure $P_{\max}$ can be obtained by using Eq. (11) at short times ($\bar{t}$ <<1), where the summation of the series becomes 1/2 and $C_{cav\to 0}^{Shirley}\cong C_0$, yielding [35]

$$P_{\max}^{Shirley}=\frac{C_0}{S_1}=RH_0P_{sat0}\frac{S_0}{S_1}=RH_0P_{sat0}\exp\left[\frac{\Delta H_s}{R}\left(\frac{1}{T_0}-\frac{1}{T_1}\right)\right]. \tag{12}$$

Eq. (12) can be rewritten by approximating P_{sat} using the Clausius–Clapeyron (CC) equation [35, 36, 51]:

$$P_{sat}=P_\infty\exp\left(-\Delta H_{vap}/(RT)\right) \tag{13}$$

with P_∞ =3.8208×10^{10} Pa and $\Delta H_{vap}\approx 40.2\times 10^3$ J/mol by fitting the steam table in [52]. Substituting Eq. (13) into Eq. (12) yields

$$P_{\max}^{Shirley}=RH_0P_\infty\exp\left[\frac{\Delta H_s-\Delta H_{vap}}{RT_0}-\frac{\Delta H_s}{RT_1}\right]. \tag{14}$$

Eq. (14) indicates that $P_{\max}$ is proportional to RH_0, and weakly dependent on T_0 if the difference between ΔH_s and ΔH_{vap} is small. For a typical epoxy molding compound [35], $\Delta H_s=38.7$

kJ/mol, so $\Delta H_s - \Delta H_{vap} \approx -1.5$ kJ/mol. The results in Fig. 4 showed that the resulting $P_{\max}$ is significantly lower than P_{sat1}, and more accurately lower than the product of P_{sat1} and RH_0. This, however, could be directly explained from Eq. (14). More discussions will be provided in Section 2.6.

2.2 Hui's Solution

Hui et al. [36] conducted another analytical study on a similar problem illustrated in Fig. 5. An isolated crack-like cavity was assumed in the middle of a moisture permeable material. Due to the symmetry in geometry, the 1-D problem can be stated exactly the same as the problem studied in [36]. Similar assumptions are also adopted, including the neglect of solid deformation and uncoupling with thermal diffusion. However, the methods used in the two works are different.

The same diffusion equation as stated in Eq. (4) was normalized and solved in [36]. However, an integral form of the boundary condition at $x=w$ is used

$$1 - g(X = \alpha, \tau > 0) = \omega_1 - \int_0^{\tau} \frac{\partial g}{\partial X}(X = \alpha, \tau')d\tau' \tag{15}$$

where the normalized variables are: $g=1-C/C_0$, $X = d\omega_1 x / l$, $\alpha = d\omega_1 w / l$, $\tau = d^2\omega_1^2 D_1 t / l^2$, $d = R_w C_0 T_0 / P_{sat0}$, and $\omega_1 = T_1 P_{sat0} / (T_0 P_{sat1})$. Eq. (15), in fact, is an integration form of Eq. (7) and Eq. (8).

Applying Laplace transformation and residual theorem, [36] obtained the exact solution to normalized concentration g at cavity surface, as

$$g(X = \alpha, \tau) = g_0 + \sum_{n=0}^{\infty} 2\exp(-\frac{u_n^2 \tau}{\alpha^2}) \frac{(1-\omega_1)\sin(u_n)/u_n - g_0\alpha / u_n^2}{(1+\alpha)\sin(u_n)/u_n + \cos(u_n)} \tag{16}$$

where $g_0 = 1 - C_1 / C_0$ and u_n is the roots of $u\tan(u) = \alpha$.

Then the cavity pressure was calculated by utilizing Eq. (3) based on Henry's law, as

$$\frac{P_{cav}^{Hui}(\tau)}{P_{sat1}} = 1 - g(X = \alpha, \tau)\,. \tag{17}$$

Eq. (17), however, is only valid for $k_H(T_0) = k_H(T_1)$ and RH_0=100% [36, 42]. To gain an insight into the assumption, we re-write k_H by replacing P_{sat} with the CC equation in Eq. (13), obtaining

$$k_H(T) = \frac{1}{P_{sat}S} = \frac{1}{p_\infty S_\infty}\exp\left(\frac{-\varDelta H_s^*}{RT}\right) \tag{18}$$

where $\varDelta H_s^* = \varDelta H_s - \varDelta H_{vap}$ called the net isosteric heat of sorption. Eq. (18) indicates that the assumption $k_H(T_0) = k_H(T_1)$ is used in Hui's solution corresponding to the case of $\varDelta H_s^* = 0$ kJ/mol.

The form of Hui's solution is apparently different from Shirley's solution given in Eq. (10). In addition, parameters in [36] were set as RH_0 =100% and $\varDelta H_s^*$=0 kJ/mol, whereas in [35], RH_0 =85% and only $\varDelta H_s^*$=-1.5 kJ/mol was applied to represent the property of typical epoxy molding compound. In the following, we provide a generalized and unified solution, which is applicable to any choice of material parameters.

2.3 Chen's Solution

Chen et al. [42] presented a vapor pressure solution with temperature-dependent Henry's law for moisture sorption for both infinitely-rapid heating and step heating profiles. For temperature-dependent k_H given by Eq. (18) and varying RH_0, Chen's solution states

$$\frac{P_{cav}^{Chen}(\tau)}{P_{sat1}} = \frac{k_H(T_1)}{k_H(T_0)}\cdot RH_0 \cdot \left(1 - g(X = \alpha, \tau)\right) = \exp\left[\frac{\varDelta H_s^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right]\cdot RH_0 \cdot \frac{C_{cav}^{Chen}(\tau)}{C_0} \tag{19}$$

where g is obtained from Eq. (16) and $C_{cav}^{Chen}(\tau) = C_0(1 - g(X = \alpha, \tau))$.

In the case of the infinitely large geometry (i.e., $w \to \infty$) , the solution of Eq. (19) can be reduced to [36, 42]

$$\frac{P_{cav}^{Chen}(\tau; w \to \infty)}{P_{sat1}} = \exp\left[\frac{\Delta H_s^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \cdot RH_0 \cdot \left[1 - \left(1 - \omega_1\right)\exp\tau \times erfc\tau\right] \tag{20}$$

For another special case of the "zero-size" cavity, when a different set of normalized variables are used: $\bar{x} = x / w$ and $\bar{t} = D(T_1)t / w^2$, the solution to g in Eq. (20) becomes [42]

$$1 - g(\bar{x}, \bar{t}; l \to 0) = \frac{C_{cav \to 0}^{Chen}}{C_0} = \frac{C_1}{C_0} + \left(1 - \frac{C_1}{C_0}\right)\sum_{n=0}^{\infty} 2\frac{\left(-1\right)^n}{u_n}\cos\left(u_n \bar{x}\right)\exp\left(-u_n^2 \bar{t}\right) \tag{21}$$

where $\gamma_n=(2n+1)\pi/2$. Eq. (21) indeed resembles with Eq. (11), yielding $C_{cav \to 0}^{Chen} = C_{cav \to 0}^{Shirley}$. The corresponding pressure solution for zero-size cavity is

$$\frac{P_{cav \to 0}^{Chen}}{P_{sat1}} = k_H(T_1) \cdot C_0 \cdot \frac{C_{cav \to 0}^{Chen}}{C_0} = \exp\left[\frac{\Delta H_s^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \cdot RH_0 \cdot \frac{C_{cav \to 0}^{Chen}}{C_0} \tag{22}$$

It is worth noting that the Chen's solution in Eq. (19) and its special solutions in Eqs. (20) and (22) have the same mathematical form except for the difference in the concentration term.

As a comparative study, Fig. 6 plots the numerical results of Shirley's solution, Hui's solution and Chen's solution with different material properties. With RH_0=100% and $\Delta H_s^* = -1.5$ kJ/mol, Chen's solution matches Shirley's solution exactly. With RH_0=100% and $\Delta H_s = 40.2$ or ΔH_s^*=0.0 kJ/mol, Chen's solution matches exactly with Hui's solution that assumes temperature-independent k_H. Therefore, Chen's solution provides a unified and general solution for vapor pressure calculation under the assumption of linear and temperature-dependent Henry's law. Discussions of additional important results obtained from Chen's solution will be described in Sec. 2.6.

2.4 Wong's Equation

Wong *et al.* [34] reported another formula to calculate the water vapor pressure in a cavity or delamination, as

$$P_{cav}^{Wong} = P_0 W_d \cdot \exp\left[\frac{\Delta H_s}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \tag{23}$$

where $W_d = C_{cav} / C_{sat}$, where C_{sat} is saturated moisture concentration for a given RH. Eq. (23) assumes that there is no moisture diffusion into the nonexpendable cavity [34]. Therefore, it applies that $C_{cav} = C_{cav\to 0}^{Shirley} = C_{cav\to 0}^{Chen}$ and $C_{sat} = C_0$ for the 1-D problem. Dividing Eq. (23) with P_{sat1} yields:

$$\frac{P_{cav}^{Wong}}{P_{sat1}} = \exp\left[\frac{\Delta H_s^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] RH_0 \frac{C_{cav\to 0}^{Chen}}{C_0} = \frac{P_{cav\to 0}^{Chen}}{P_{sat1}}. \tag{24}$$

Eq. (24) indicates that Wong's equation is a special case of Chen's solution by assuming zero-size cavity.

2.5 Bhattacharyya's Equation

Bhattacharyya *et al.* [43] proposed an empirical equation based on thermodynamics and the assumption of no moisture diffusion during the heating, as

$$P_{cav}^{Bhatt}(T_1) = R_w T_0 RH_0 \rho_g(T_0) \exp\left[2740\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \tag{25}$$

where $\rho_g(T) = P_{sat}(T) / R_w T$. Notice that $R_w T_0 RH_0 \rho_g(T_0) = P_{sat0} RH_0$ based on ideal gas law and Henry's law, so Eq. (25) can be rewritten as

$$\frac{P_{cav}^{Bhatt}}{P_{sat1}} = \exp\left[\left(2740 - \frac{\Delta H_{vap}}{R}\right)\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \cdot RH_0 = \exp\left[\left(2740 - \frac{\Delta H_s}{R}\right)\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \cdot \frac{P_{\max}^{Chen}}{P_{sat1}}. \tag{26}$$

Therefore, Bhattacharyya's equation becomes the solution of $P_{\max}^{Chen}$ if $\Delta H_s = 2740 R = 22.78$ kJ/mol or $\Delta H_s^* \approx$ -17.4 kJ/mol.

2.6 Discussions

Chen's solutions in Eqs. (19), (20), and (22) have the following unified form:

$$\frac{P_{cav}^{Chen}}{P_{sat1}} = \exp\left[\frac{\Delta H_s^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] RH_0 \frac{C_{cav}}{C_0} \tag{27}$$

where C_{cav} is moisture concentration in the cavity (e.g., for a zero-size cavity, $C_{cav} = C_{cav\to 0}$). Eq. (27) can be considered as a unified equation of Shirley's solution, Hui's solution, Wong's equation, and Bhattacharyya's equation (after certain transformations). The unified solution for the maximum pressure can be obtained by letting $C_{cav} = C_0$ in Eq. (27), as [42]

$$\frac{P_{\max}^{Chen}}{P_{sat1}} = \exp\left[\frac{\Delta H_s^*}{R}\left(\frac{T_1 - T_0}{T_0 T_1}\right)\right] RH_0 . \tag{28}$$

Eq. (28) can be derived by dividing $P_{\max}^{Shirley}$ in Eq. (10) with P_{sat1}, indicating that they represent the same solutions. Unlike Shirley's equation in Eq. (10), Chen's or unified solution in Eq. (28) gives an explicit relation between $P_{\max}$ and P_{sat1}. Some important implications of Eq. (28) are discussed as follows.

2.6.1 *Effect of* RH_0

To demonstrate the effect of RH_0, Fig. 7 plots the normalized cavity pressure, P_{cav}/P_{sat1}, versus normalized time, τ, under different various values of parameter, α (see definitions of τ and α in Eq. (15)). Generally, the pressure experiences a rapid increase at the early stage of heating, but gradually decreases due to moisture loss. The maximum pressure increases as α increases (or thickness increases), reaching the solution for $w=\infty$ given in Eq. (20) when $\alpha>100$. However, Fig. 7 also shows that the normalized pressure is significantly lower than RH_0 (a dashed horizontal line in the figure) even for $\alpha=\infty$. This is considered as the capping effect of RH_0, meaning that the maximum vapor pressure could not surpass the product of saturated vapor pressure and RH_0 for the given parameter settings (i.e., $\Delta H_s^* = -1.5$ kJ/mol). The effect of different ΔH_s^* is further discussed in the following.

2.6.2 *Effect of* ΔH_s^*

Figure 8 plots the normalized cavity pressure for negative, zero, and positive values of ΔH_s^*. As ΔH_s^* increases from a negative value to zero, the normalized pressure could approach to but never exceed RH_0. However, when ΔH_s^* is a positive value (i.e., ΔH_s^* = 3.0 kJ/mol), the normalized pressure surpasses RH_0 and may become even greater than 1.0 after τ>5.0. This means that the cavity pressure is higher than P_{sat1}. Although the saturated vapor pressure represents the maximum water vapor pressure at a particular temperature, with a positive value of ΔH_s^*, the predicted vapor pressure can be greater than the saturated water vapor pressure.

Mathematically, the following three different scenarios for a heating process (T_1>T_0) can be obtained from Eq. (28), as:

$$\frac{P_{\max}^{Chen}}{P_{sat1}}\begin{cases} < RH_0, & \Delta H_s^* < 0 \\ = RH_0, & \Delta H_s^* = 0 \\ > RH_0, & \Delta H_s^* > 0 \end{cases} \cdot \tag{29}$$

Literature shows that ΔH_s^* could range from -5.0 kJ/mole for microcrystalline [49, 53] and 6.0 kJ/mole for certain epoxy network [54]. Therefore, all the three scenarios in Eq. (29) can occur. Bhattacharyya's equation even adopted an extreme case with ΔH_s^*≈-17.4 kJ/mol.

Figure 9 plots $P_{\max}/P_{sat1}$ versus a wide range of ΔH_s^* from -5.0 to 6.0 kJ/mol. Two reflow temperatures (T_1) are compared, which shows that the dependence or sensitivity of cavity pressure on ΔH_s^* increases as T_1 increases. Generally, when $\Delta H_s^* \le 0$, cavity pressure is restricted by RH_0 (=85%), or $P_{\max} \le P_{sat1} \cdot RH_0$. The results that were given in Shirley's solution, Hui's solution, and Bhattacharyya's equation fall into this category. However, when $\Delta H_s^* > 0$, it becomes possible to exceed the saturated vapor pressure. For example, if ΔH_s^* =2.0 kJ/mol, the maximum cavity pressure reaches saturated vapor pressure P_{sat1} at T_1=215 °C even RH_0<100%. Above ΔH_s^* (=2.0

kJ/mol) there exists unphysical pressure greater than P_{sat1}. The findings of capping effect of RH_0 as well as unphysical pressure, pose a great challenge for using the water vapor pressure models based on the linear sorption isotherm or Henry's law.

3. VAPOR PRESSURE MODELS CONSIDERING VAPOR FLOW

3.1 Convection-only Model

Water vapor pressure models reviewed in Sec. 2 only consider moisture transport through diffusion during rapid heating. At elevated temperature, however, convective vapor flow may become dominant over diffusion for a porous media. Consider a special case where vapor flow is the only mechanism for moisture transport at higher temperature, a "convection-only" model is then developed to describe the vapor flow during rapid heating [37]

$$\left[\frac{\phi}{R_w T}+(1-\phi)\frac{K_H}{P_{sat}}\right]\frac{\partial P_v}{\partial t}-\frac{\kappa}{\mu R_w T}\nabla\cdot(P_v\nabla P_v)=\left[\frac{\phi}{R_w T^2}+\frac{(1-\phi)K_H}{P_{sat}^2}\frac{dP_{sat}}{dT}\right]\dot{T}P_v \tag{30}$$

where P_v is vapor pressure (in pores), ϕ is porosity, K_H is Henry solubility constant (=$1/k_H$ when ΔH_s^*=0 kJ/mol), κ is Darcy's vapor permeability, μ is vapor viscosity, and $\dot{T}$ is the heating rate. Since the porosity is introduced, vapor pressure at any location in media may be calculated. The above formulation, however, does not consider material deformation, which is consistent with the model assumptions in Sec. 2. Eq. (30) may be solved numerically using finite difference method.

The convection-only model can be applied to the 1-D problem depicted in Fig. 5 in Sec. 2. The equivalent porosity is calculated as $\phi_{eq}= l/(w+l)$, and vapor permeability is set to be $\kappa=1.1\times10^{-20}$ m^2 based on [44]. The Henry solubility constant is calculated as $K_H=1/k_H=20.85$ kg/m^3. Since K_H or k_H is temperature-independent, it is valid that $\Delta H_s^* = 0$ kJ/mol. The stepping temperature change is approximated with a high heating rate (i.e., $\dot{T}$ =10000 K/sec). Fig. 10 compares Chen's analytical solution and numerical solution of the convection-only model with l=0.01 cm and w=0.2 cm (i.e.,

ϕ_{eq}=0.5%). Different results are obtained from the two models, mainly due to the difference of transport mechanism between moisture diffusion and vapor convection. The maximum pressure based on the convection-only model is slightly lower than Chen's solution. The similarity between the two different models is due to the use of the same Henry's law.

3.2 Convection-Diffusion (CD) Model

A more general porous media model has been developed by [44] to consider both moisture diffusion in the bulk material and vapor flow in the pores, as schematically shown in Fig. 11. In this model, water is partitioned into two different states: one is in vapor form that flows through pore network, and the other is in liquid form that is dissolved into a solid matrix. Considering both the vapor convection and moisture diffusion mechanism, the final governing equation in solving pore vapor pressure is [44]:

$$\frac{\phi}{R_w}\frac{\partial(P_v/T)}{\partial t}+(1-\phi)\frac{\partial(K_H P_v/P_{sat})}{\partial t}=\frac{\kappa}{\mu R_w T}\nabla\cdot(P_v\nabla P_v)+\frac{K_H D}{P_{sat}}\nabla^2 P_v \cdot \tag{31}$$

where P_v is vapor pressure (in pores), ϕ is porosity, K_H is Henry solubility constant (=1/k_H when ΔH_s^*=0 kJ/mol), κ is Darcy's vapor permeability, μ is vapor viscosity, D is diffusivity, and $\dot{T}$ is the heating rate.

The CD model in Eq. (31) was applied to study water vapor pressure within the sample of epoxy molding compound in [44]. The problem is similar to the 1-D problem in Fig. 5 (without considering the "cavity" in the middle). The material is initially saturated at RH=85% at T=300 K and is heated to 600 K at a rate of 1 K/s. Fig. 12 compares water vapor pressure results for three different cases: convection-diffusion, convection only, and diffusion only, respectively. The heating process stops at t=300 seconds, so there exists a turning point for all the curves of vapor pressure results. The diffusion-only model gives a pressure up to two times higher than that given by the CD model, while the convection-only model predicts a pore pressure lower than the CD model. This is mainly because the diffusion-only model ignores the vapor flow at high temperatures and results in a slower desorption for the buildup of pore pressure, whereas the convection-only model overestimates the vapor flow by using a higher vapor permeability κ (=1.1×10^{-20} m^2) than CD model (κ=6.9×10^{-21} m^2) and results in faster desorption and lower vapor pressure [44]. Generally, the CD model or convection-only model predicts a lower pressure because the interconnected pore network within porous media provides another fast path for moisture transport in the form of vapor flow.

To consider temperature-dependent K_H in CD model, Eq. (31) has been further extended to as [45]

$$\left[\frac{\phi}{R_w T}+(1-\phi)\frac{K_H(T)}{P_{sat}}\right]\frac{\partial P_v}{\partial t}=\nabla\cdot\left(\frac{\kappa P_v \nabla P_v}{\mu R_w T}+\frac{K_H(T) D \nabla P_v}{P_{sat}}\right)+\left[\frac{\phi}{R_w T^2}+\frac{(1-\phi)K_H(T)}{P_{sat}^2}\frac{dP_{sat}}{dT}-\frac{(1-\phi)}{P_{sat}}\frac{dK_H(T)}{dT}\right]\dot{T}P_v \tag{32}$$

where K_H=$K_H(T)$. With this model, the moisture “overshooting” at the material interface, as reported in [28, 40], has been simulated in [45]. The numerical studies in [45] also showed that the vapor pressure predicted from the model in Eq. (32) correlated well with experimental observations of cohesive failures of polymer thin films in a stacked-chip microelectronic package .

4. GENERALIZED FRAMEWORKS TO CONSIDER NONLINEAR SORPTION ISOTHERMS

4.1 Nonlinear Moisture Sorption Models

Vapor pressure models in previous Sec. 2 and Sec. 3 are based on Henry’s law, which assumes a linear and temperature-dependent relationship between saturated moisture concentration C_{sat} and ambient relative humidity RH_{amb}. However, moisture permeable material may exhibit nonlinear moisture sorption behavior. As shown in Fig. 13, there are five typical types of moisture absorption curves to describe the relationship between C_{sat} and ambient water activity (which is denoted as $a_{w,eq}$ and is equal to RH_{amb}) . These sorption isotherms include Henry sorption, nonlinear sorption for hydrophobic materials [55, 56], Langmuir sorption [57, 58], nonlinear sorption for high water interaction [59], and sigmoidal sorption curve [60].

Table 1 lists some existing mathematical models to describe the moisture sorption isotherms (the temperature effect is not included in those models). In the following, two generalized frameworks are developed to evaluate vapor pressure with the consideration of these nonlinear functions.

Table 1. Mathematical models for nonlinear water sorption isotherms [61]. p_i is are the model parameters; $a_{w,eq}$ is equilibrium or ambient water activity.

Model Name	Mathematical expression
Henry's law	$C_{sat}=p_1 a_{w,eq}$
Dual sorption model [62]	$C_{sat} = p_1 a_{w,eq} + \frac{p_2 \cdot p_3 \cdot a_{w,eq}}{1 + p_2 \cdot a_{w,eq}}$
GAB [63]	$C_{sat} = p_1 a_{w,eq} + \frac{p_1 p_2 p_3 \cdot a_{w,eq}}{(1 - p_3 a_{w,eq})(1 - p_3 a_{w,eq} + p_2 p_3 a_{w,eq})}$
Henderson-Thompson	$C_{sat} = \left(\frac{\ln(1 - a_{w,eq})}{- p_1 (T + p_2)} \right)^{1/p_3}$
Modified Chung-Pfost	$C_{sat} = p_1 - p_2 \ln(a_{w,eq}) \ln(-T + p_3)$
Chirife and Iglesias	$C_{sat} = p_1 + p_2 a_{w,eq} + p_3 (a_{w,eq})^2 + p_4 (a_{w,eq})^3$
Halsey	$C_{sat} = p_1 \left(- \frac{p_2}{\ln(a_{w,eq})} \right)^{1/k_3}$
Oswin	$C_{sat} = p_1 \left(\frac{a_{w,eq}}{1 - a_{w,eq}} \right)^{1/p_2}$
Peleg	$C_{sat} = p_1 (a_{w,eq})^{p_2} + p_3 (a_{w,eq})^{p_4}$
Smith	$C_{sat} = p_1 + p_2 \cdot \log(1 - a_{w,eq})$
Caurie	$C_{sat} = \exp\left[a_{w,eq} \ln(p_1) - \frac{1}{4.5 p_2} \right]$
Ferro Fontan	$C_{sat} = p_1 \left(\ln \frac{p_2}{a_{w,eq}} \right)^{p_3}$

4.2 A Concentration-Based Framework

Let the moisture diffusion within solid matrix be considered by Fick's second law as given in Eq. (4). A general function f_C is applied at the material interface and cavity surface, as $C_{sat}=f_C(a_{w,eq}, T)$ to describe the nonlinear isotherm. The cavity pressure then can be evaluated by

$$P_{cav} = a_{w,cav} P_{sat}(T) = f_a(C_{cav}, T) P_{sat}(T) \tag{33}$$

where $a_{w,cav} = f_a(C_{cav}, T)$ and $f_a = f_C^{-1}$. Accordingly, the initial and boundary conditions are changed to

$$\begin{cases} C(x, t=0) = f_C(RH_0, T_0) = C_0 \\ C(x=0, t) = f_C(RH_1, T_1) = C_1 \\ C(x=w, t=0+) = f_C(\dfrac{P_0 T_1}{P_{sat1} T_0}, T_1) \\ \dfrac{lP_{sat1}}{R_w T_1} \dfrac{\partial f_a(C, T_1)}{\partial C} \dfrac{\partial C}{\partial t} + D_1 \left.\dfrac{\partial C}{\partial x}\right|_{x=w} = 0 \end{cases} \tag{34}$$

where the values of $a_{w,eq}$ for initial and reflow conditions are equal to RH_0 and RH_1, respectively. It is interesting to notice that Eq. (34) will be independent of the function f_C for the special case of zero-size cavity, as long as the same C_0 and C_1 are used. In other words, the same solution to $C_{cav\to 0}$ as given in Eq. (11) would apply to all types of sorption models. However, the cavity pressure $P_{cav\to 0}$ will still depend on the sorption function f_C.

The corresponding maximum pressure will be obtained with $C_{cav\to 0} = C_0$, as

$$P_{\max} = P_{sat1} f_a(C_0, T_1). \tag{35}$$

To compare with the solutions based on Henry's law, one can transform Eq. (35) through the Clausius-Clapeyron (CC) relation in Eq. (36) [64-67]:

$$a_{w0} = a_{w1} \exp\left[\frac{Q_{st}^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \tag{36}$$

where $a_{w0} = f_a(C_0, T_0) = RH_0$, $a_{w1} = f_a(C_0, T_1)$, $Q_{st}^* = Q_{st} - \Delta H_{vap}$, and Q_{st} is the isosteric heat of sorption. Note that $Q_{st}^* = \Delta H_{sol}^*$ for Henry's law. Subsisting Eq. (36) into Eq. (35) yields $P_{\max}^{conc}$, the maximum pressure based on the concentration-based framework:

$$P_{\max}^{conc} = P_{sat1} RH_0 \exp\left[\frac{Q_{st}^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] \tag{37}$$

Eq. (37), in fact, results in the same maximum pressure as Eq. (28) based on Henry's law. This indicates that the maximum pressure would be independent of the sorption models. As a result, the effects of RH_0 dependence and unphysical pressure discussed in Sec. 2.6 are applicable to both Henry's law and non-Henry sorption models.

As an example, Fig. 14 plots three different sorption isotherms: one is based on Henry's law and the other two is based on Ferro Fontan (FF) model (See Table 1). They cross at one point ($a_{w,eq}$=0.85, C_{sat}=9.781) for T=85 °C, and another point ($a_{w,eq}$=0.71, C_{sat}=9.781) for T=215 °C. Model parameters for low-temperature are given, and the high-temperature isotherms are derived using the CC relation in Eq. (36) with $Q_{st} = 38.7$ kJ/mol or $Q_{st}^* = -1.5$ kJ/mol. The three different isotherms can be applied to calculate water vapor pressure by solving Eqs. (4), (33) and (34). The results are compared in Fig. 15 where both the moisture concentration and cavity pressure are plotted for a zero-size cavity problem according to [35]. It can be seen that moisture concentration deviates greatly due to the difference in the sorption isotherm, but the cavity pressure is the same at the early stage and only deviates slightly at a later time. The maximum pressure is lower than P_{sat1} at 215 °C due to the use of a negative Q_{st}^*, which is consistent with Eq. (37).

4.3 An Activity-Based Framework

The vapor pressure models previously discussed utilize concentration-based diffusion theory described by Fick's second law. A more fundamental equation for moisture diffusion is based on the gradient of chemical potential, as [68, 69]

$$\begin{cases} \mathbf{J} = -CB\nabla\mu_w; \\ \partial C/\partial t = -\nabla\cdot\mathbf{J} \end{cases} \tag{38}$$

where **J** is water flux, *B* is mobility of water molecules, and μ_w is water chemical potential that can be written as [68]

$$\mu_w = \mu_{w0} + RT\ln a_w \tag{39}$$

where μ_{w0} is reference chemical potential.

Introducing the generalized solubility *K* as [36, 68, 70]:

$$K = C/a_w \tag{40}$$

and assuming a uniform temperature (or ∇T =0), one can obtain a general, activity-based diffusion theory, as [70]

$$\left(K + a_w\frac{\partial K}{\partial a_w}\right)\frac{\partial a_w}{\partial t} = \nabla\cdot\left(KD\nabla a_w\right) - a_w\frac{\partial K}{\partial T}\frac{\partial T}{\partial t} \tag{41}$$

in which moisture diffusivity *D*=*BRT*. Because water activity is a state variable and always continuous, the activity-based model in Eq. (41) does not require normalization at the material interface. This is convenient for studying multi-material systems where the concentration-based model must be normalized due to the concentration discontinuity. It was also found that Eq. (41) returns to Fick's second law under the assumption of Henry's law [70].

The generalized solubility *K* in Eq. (41) is a material property that can be evaluated from the sorption function f_c , as

$$K = C_{sat} / a_{w,eq} = f_c(a_{w,eq}, T) / a_{w,eq} \tag{42}$$

where function f_c can be given by Table 1 and the CC relation in Eq. (36). With K determined, the initial and boundary conditions for Eq. (41) are changed to

$$\begin{cases} a_w(x, t=0) = RH_0 \\ a_w(x=0, t) = RH_1 \\ a_w(x=w, t=0+) = P_0 T_1 / \left(P_{sat1} T_0\right) \cdot \\ \left. \dfrac{lP_{sat1}}{R_w T_1} \dfrac{\partial a_w}{\partial t} + D_1 \dfrac{\partial \left(K a_w\right)}{\partial x} \right|_{x=w} = 0 \end{cases} \tag{43}$$

which may be solved by numerical approaches. Once the water activity is solved, cavity pressure is readily obtained by using the relationship $P_{cav}=P_{sat}\cdot a_{w,cav}$.

To derive the maximum vapor pressure, consider a sufficiently short period of time when the moisture concentration at the cavity remains to be C_0. In this case, the following relationship holds at cavity surface:

$$K(T_0, a_{w0}) a_{w0} = K(T_1, a_{w1}) a_{w1} \equiv C_0, \tag{44}$$

where a_{w0} and a_{w1} are the water activity corresponding to C_0 at T_0 and T_1, respectively. Applying Eq. (36) to Eq. (44) leads to

$$\frac{K(T_0, a_{w0})}{K(T_1, a_{w1})} = \frac{a_{w1}}{a_{w0}} = \exp\left[\frac{Q_{st}^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right]. \tag{45}$$

The maximum pressure is corresponding to a_{w1} and can be written as

$$\frac{P_{\max}^{aw}}{P_{sat1}} = a_{w1} = \frac{K(T_0, a_{w0})}{K(T_1, a_{w1})} a_{w0} = \exp\left[\frac{Q_{st}^*}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right] RH_0 = \frac{P_{\max}^{conc}}{P_{sat1}} \tag{46}$$

Eq. (46) shows that the two frameworks proposed in this paper give a consistent solution and $P_{\max}$ is independent of moisture sorption isotherms.

5. MICROMECHANICS-BASED VAPOR PRESSURE MODELS

Micromechanics-based vapor pressure models are reviewed as follows, including the two-phase micromechanics-based model, the one-phase semi-infinite medium model, and other empirical models. They are also compared with Henry's law-based models reviewed in Sec. 3.

5.1 Two-Phase Micromechanics-Based Model

Fan *et al.* [39] developed a micromechanics-based vapor pressure model, or Fan's model, to calculate water vapor pressure in moisture permeable material. A representative elementary volume (REV) is taken from the material, as shown in Fig. 16. It assumes that the total volume of the studied REV can be divided into the free volume or microvoids, where moisture resides, and the occupied volume for the solid only. The porosity ϕ in REV defines the collective free volume or microvoids. In the micromechanics-based model, moisture only resides in microvoids with two possible states or phases: a pure vapor phase or a mixed phase with both liquid and vapor, as shown in Fig. 16.

Introduce the apparent moisture density ρ_a, as

$$\rho_a = C(x,t)/\phi \quad . \tag{47}$$

Phase transition of water vapor occurs when ρ_a reaches the saturated vapor density, or $\rho_g = P_{sat}/(R_w T)$. If the apparent density ρ_a is smaller than ρ_g, only the vapor phase exists, otherwise the moisture is in a mixed phase. Therefore, water vapor pressure in a microvoid can be evaluated by

$$P_v^{Fan}(T) = \begin{cases} \dfrac{R_w T}{\phi} \cdot C(x,t), & \rho_a < \rho_g(T) \\ P_{sat}(T), & \rho_a \geq \rho_g(T) \end{cases} \quad . \tag{48}$$

To use this model, $C(x,t)$ is first solved based on applicable diffusion theory (i.e., Fickian or non-Fickian models reviewed in [71]). Then water vapor pressure can be evaluated with Eq. (48). Applications and more discussions on the micromechanics-based models can be found in [38-40].

To compare this model with Henry's law based models, a cavity problem defined in Fig. 3 is revisited. The equivalent porosity is computed as $\phi_{eq} = l/(w+l)$ similar to the use of the convection-only model in Sec. 3. The results are given in Fig. 17, where Chen's unified solution in Eq. (27) is also plotted for comparison. It can be seen that Fan's model predicts a pressure staying at the saturated vapor pressure for the most time of the heating process. However, Chen's analytical solution, which is based on temperature-dependent Henry's law with a negative ΔH_s^* (= -1.5 kJ/mol), gives much lower vapor prediction.

5.2 Alpern's One-Phase Model

Alpern *et al.* [46] proposed a model for calculating the water vapor pressure in a semi-infinite body with a cavity. It assumes that all the absorbed moisture is driven into the cavity during the diffusion process. An analytical equation was derived to calculate the amount of moisture entering into the cavity [46]:

$$M(t) \approx C_0 A \sqrt{(4/\pi) D_1 t} \tag{49}$$

where *A* is the body surface. It also assumed that moisture accumulated in the cavity is always in vapor form and never condenses. Applying the ideal gas law yields

$$P_{cav}^{Alpern}(t) = M(t) R_w T_1 / V \tag{50}$$

where *V* is the volume of the cavity. Using the elastic plate theory for both rectangular and cylindrical semi-infinite bodies, the relationship between the cavity pressure and *V* can be obtained [46]. Alpern's model is basically a one-phase model without considering the phase change of water vapor. For the 1-D problem, Alpern's equation yields the following equation for cavity pressure:

$$P_{cav}^{Alpern}(w \to \infty, t) = C_0 \sqrt{\frac{(4/\pi) D_1 t}{l^2}} R_w T_1 \tag{51}$$

Figure 18 compares Alpern's solution with Fan's model and Henry's law-based solution. It can be seen that Alpern's one-phase model yields much higher pressure than the other two solutions when the cavity size is small, far beyond the saturated vapor pressure.

5.3 Sawada's Model

Sawada [72] proposed the following empirical equation for calculating water vapor pressure in cavity/delamination:

$$P_{cav}^{Sawada}(T_1) = \min\left[G_1 \cdot C_0 \cdot T_1 \quad , \quad P_{sat}(T_1) \cdot RH_0\right] \tag{52}$$

where G_1 is an empirical constant. Similar empirical equations were also used in other works [73, 74]. The use of Sawada's and other similar equations, however, is very limited because G_1 is usually unknown and is difficult to determine through experiments.

6. A MODIFIED FAN'S MODEL

6.1 Consideration of Capillary Effect in Microvoids

According to Kelvin's equation, the saturation point may be altered by capillary effect for small-size voids [75-77]

$$\ln \frac{P'_{sat}}{P_{sat}} = -\frac{2\sigma V_m \cos\theta}{rRT} \tag{53}$$

where P'_{sat} is modified vapor pressure at phase change, σ is surface tension of water, V_m is water molar volume (0.018 L/mol), θ is the surface wetting angle for the pore surface, and r is pore radius. Eq. (53) assumes a cylindrical shape of the pore. For a perfect wetting condition, $\theta = 0^{\circ}$.

Based on Eq. (53), the corresponding saturated vapor density for a microvoid with a size of r should be modified as

$$\rho'_g(r,T) = \frac{P'_{sat}(r,T)}{R_w T} = \frac{P'_{sat}(r,T)}{P_{sat}} \rho_g(T) \,. \tag{54}$$

A modified Fan's model thus can be obtained:

$$P_{cav}^{Fan+}(T) = \begin{cases} \dfrac{R_w T}{\phi} \cdot C(x,t), & \rho_a < \rho'_g(r,T) \\ P'_{sat}(r,T), & \rho_a \ge \rho'_g(r,T) \end{cases} \,. \tag{55}$$

6.2 Case Study

To investigate capillary effect, various void sizes and water surface tension coefficients at different temperatures are considered. The pore radius ranges from 0.1~100 nm based on typical values for polymeric materials[78]. Both constant surface tension (σ_{rm} =0.072 N/m, [79-81]) and temperature-dependent surface tension are considered. For the latter, the temperature-dependent σ can be evaluated by the following linear equation:

$$\sigma(T) = \sigma_{rm} - 0.0002 \times (T - 293.15) \tag{56}$$

which simulates about 85% decrease of surface tension at 600 K according to the atomic studies in [82]. Fig. 19 shows the ratio of P'_{sat}/P_{sat} under various temperatures. Perfect wetting is considered with θ=0°. When a constant surface tension is used, the capillary effect on the ratio of P'_{sat}/P_{sat} is significant as shown in Fig. 19a. On the other hand, for temperature-dependent σ described by Eq. (56), the capillary effect becomes less significant at high temperatures as seen from Fig. 19b.

Figure 20 presents the vapor pressure results of modified Fan's model for the 1-D problem of a step change from 85 °C to 215 °C. The solution of moisture concentration is obtained on an equivalent porosity of 5% using the diffusion parameters given in [35]. Various void sizes are compared, with r=0.5 nm, 1.0 nm, 10 nm and ∞. It can be proved that the original Fan's solution is obtained at r=∞ when capillary effect vanishes. However, when a very small void size is considered (e.g., 0.5 nm), the maximum vapor pressure drops by 75% for a constant surface tension and 50%

for temperature-dependent surface tension. Like original Fan's model, the unphysical pressure will not occur in the modified Fan's model with consideration of phase change and capillary effects.

7. CONCLUDING REMARKS

High vapor pressure is induced by the encapsulated moisture in moisture permeable material. The vapor pressure evolves and is coupled with moisture transport, water vapor flow, phase change, heat transfer, material's deformation, and material's microscopic change. In this paper, we present a comprehensive review of various theories and models to evaluate water vapor pressure subjected to rapid heating. In Sec. 2 and Sec. 3, Henry's law, a linear and temperature-dependent equation, is applied. Such a treatment establishes a relationship between the pressure in cavity or pores (or pore network) and the local moisture concentration in solid matrix. Even though various models provide various forms of analytical or numerical solutions, which give different results, those solutions can be unified to a general form of solution. With specific assumptions and parameter settings, the generalized solution can return to each specific solution in each model. Two key parameters appear in the unified solution for determining the magnitude of vapor pressure in cavity: the initial relative humidity RH_0, in which the material is preconditioned and saturated, and ΔH_s^*, the net solution heat, a material's property, respectively. Although the saturated vapor pressure represents the maximum water vapor pressure at a particular temperature, with a positive value of ΔH_s^*, the predicted vapor pressure can be greater than the saturated water vapor pressure. Such an "unphysical" pressure solution needs to be further studied in the future. Moreover, with a non-positive value of ΔH_s^*, the predicted maximum vapor pressure is equal to or less than the product of the saturated vapor pressure and RH_0 (≤ 1), which means that the vapor pressure is less than the saturated vapor pressure, and is directly affected by the initial relative humidity. This implies that the vapor pressure in cavity will depend on the history of moisture absorption – what initial relative humidity is applied before rapid heating, not only the present state of moisture condition.

In porous media with interconnected pore network, vapor flow provides another path for moisture transport. In this paper, two models considering vapor flow are presented, which are the so-called “convection-only” model and “convection-diffusion” model. For both models, water is partitioned into two different states: one is in vapor form that flows through pore network, and the other is liquid form that is dissolved into solid matrix. Henry’s law is applied to both external boundary and the interface between pores and solid matrix. However, the “convection-only” model considers vapor flow as dominant in moisture transport, thus diffusion is neglected. As a result of vapor flow, the predicted vapor pressure in pores or cavity by both models is generally lower than that by the models given in Sec. 2.

For materials with nonlinear sorption isotherms, two generalized frameworks: namely concentration-based and activity-based approaches, respectively, are presented in this paper. The analytical solutions for the maximum vapor pressure are derived under both frameworks. It is found that the maximum pressure is mainly governed by the net isosteric heat of sorption Q_{st}^{*} and does not depend on the types of sorption isotherms ($Q_{st}^{*} = \Delta H_{s}^{*}$ for Henry’s law).

For vapor pressure models using either Henry’s law or nonlinear sorption isotherm, the predicted vapor pressure can potentially be greater than the saturated water vapor pressure. Moreover, the predicted maximum vapor pressure is always proportional to the initial relative humidity, implying that the vapor pressure will depend on the history of moisture absorption.

For micromechanics base vapor pressure model, moisture is assumed to reside in microvoids or free volumes in material. The magnitude of the vapor pressure depends on the state or phase of moisture in voids. When moisture is in vapor phase, the vapor pressure follows the ideal gas law. When moisture is in the mixed liquid/vapor phase, vapor pressure stays at the saturated vapor pressure (Sec. 5). Furthermore, this model has been extended to take the capillary effects into consideration. It is found that considering the capillary effects will lower the predicted vapor pressure. Two completely different results are derived from the micromechanics-based model: 1). the maximum vapor pressure stays at the saturated vapor pressure provided that the moisture is in the mixed liquid/vapor phase in voids, and 2). the vapor pressure depends only on the current state of moisture condition, not a direct relationship with the initial relative humidity condition.

Material's deformation will alter the volume or size of voids or cavity during rapid heating. Therefore, to accurately evaluate vapor pressure buildup, solid or structure deformation and heat diffusion should also be considered. However, to fundamentally understand the vapor pressure theory, in particular, to obtain the analytical solutions, this paper focuses on the problems and solutions that do not consider the deformation. Also for simplicity, one-dimensional problems have been used to develop most of the analytical solutions or governing equations for determining vapor pressure. When the solid deformation is considered, numerical simulation such as coupled-field finite element analysis can be applied, but the fundamental theory of the vapor pressure presented in this paper remains same. Poroelasticity, poroplasticity, and the fully-coupled constitutive relation at a multi-scale level can be applied and integrated with vapor pressure models to fully understand the material's behavior with moisture under elevated temperature [31, 32, 83-89].

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