

# The fundamentals of thermal-mass diffusion analogy



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## ABSTRACT

The fundamentals in thermal-mass diffusion analogy are developed and the misunderstandings are clarified. The continuity of the “wetness” or, more appropriately, the “fractional saturation”,  $w = C/C_{sat}$ , is fundamentally proven using the equality principle of chemical potential. The validity of the analogy is independent of the linearity of the sorption isotherm. The mass diffusion equation with fractional saturation as the field variable is valid for source solute that is in either gaseous, liquid, or solid phase; and for absorbents that could be a combination of gaseous, liquid, and solid phases. Mass diffusion under complex conditions such as spatially non-uniform temperature and temporally varying source density/pressure can be readily modeled. However, discontinuity in fractional saturation could occur along the interface of two absorbents when diffusion occurs under a time-varying temperature condition. A novel technique – the internal source technique – has been developed that enables modeling of diffusion under such a condition using the standard thermal module in commercial finite element software.

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## 1. Introduction

Since the reported modeling of moisture diffusion in microelectronic assembly by Galloway and Miles [1] using the “partial pressure” technique inherent in the commercial finite element software, Abaqus, and the subsequent introduction of the “wetness” technique by Wong et al. [2], the modeling of moisture diffusion in microelectronic packaging using thermal-mass diffusion analogy has become a standard routine. However, the establishment of these analogical techniques have been largely based on intuition and, unfortunately, theories that are unsound. The lack of in depth understanding of the fundamentals has led to significant misunderstanding and even misapplication of these analogical techniques. It is the objective of this manuscript to develop the fundamentals of the thermal-mass diffusion analogy and to clarify the misunderstandings, which are introduced in this section.

Based on the experimental observations that the “saturated concentration of moisture” or, more appropriately, the “volumetric moisture capacity”,  $C_{sat}$  ( $\text{kg m}^{-3}$ ), differs between absorbents when exposed to the same temperature and partial pressure of water vapor, Wong et al. [2] argued that the concentration of moisture,  $C$  ( $\text{kg m}^{-3}$ ), must differ at the interface of absorbents at any stage

of diffusion. The discontinuity of field variable limits the applicability of the Fick’s laws,

$$\mathbf{J}_m = -D\nabla C \quad (1)$$

where  $\mathbf{J}_m$  ( $\text{kg s}^{-1} \text{m}^{-2}$ ) is mass flux,  $D$  ( $\text{m}^2 \text{s}^{-1}$ ) is mass diffusivity, to a domain constituting of a spatially uniform  $C_{sat}$ . Since the root cause of the discontinuity of concentration is the different magnitudes of  $C_{sat}$ , Wong et al. [2] proposed, intuitively, that the discontinuity could be removed by normalizing the effect by its cause; that is,

$$w = \frac{C}{C_{sat}} \quad (2)$$

which is referred to as “wetness fraction” or simply “wetness”. Wong et al. [2] then presented a theoretical argument for the continuity of “wetness” basing on the Henry’s law. However, the theoretical argument is flawed as the Henry’s law is invalid for solid–solid interface [3,4]. A rigorous argument of the continuity of “wetness” is desired.

Preceding the introduction of “wetness”, the pseudo partial pressure,  $p_\phi$  (Pa),

$$p_\phi = \frac{C}{K_H} \quad (3)$$

also referred to as “normalized concentration” has been adopted by Abaqus [5]. Eq. (3) takes the form of the Henry’s law

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$$p_s = \frac{C_{sat}}{K_H} \quad (4)$$

where  $p_s$  is the partial pressure of the source solute in the gaseous state and  $K_H$  ( $\text{kg m}^{-3} \text{Pa}^{-1}$ ) is the Henry's coefficient [3,4], which is a property of the solute-absorbent system. It is worth noting that in the theory manual of Abaqus [5], the symbol  $s$ , referred to as “solubility”, is used in place of the Henry's coefficient ( $K_H$ ); this is unconventional and the conventional use of Henry's coefficient is restored in this manuscript. The continuity of  $p_\phi$  is argued using the claimed continuity of the pseudo partial pressure,  $p_\chi$  (Pa),

$$p_\chi^{1/2} = \frac{C}{s} \quad (5)$$

which takes the form of the Sievert's law [6],

$$p_s^{1/2} = \frac{C_{sat}}{s} \quad (6)$$

where  $s$  ( $\text{kg m}^{-3} \text{Pa}^{-0.5}$ ) is the solubility of a diatomic gas in a metal absorbent (remark: the two different definitions of solubility defined by Abaqus is indeed rather confusing). Both  $p_\chi$  and  $p_\phi$  are referred to as pseudo partial pressure in that they are an artificial extension of the partial pressure of the gaseous solute in a gaseous mixture into the solid absorbent wherein the concept of partial pressure does not apply – unless the solid absorbent has the characteristic of a perfect gas. Therefore, the claimed continuity of  $p_\chi$  and hence  $p_\phi$  are unsupported.

A question that would have naturally come to the mind of those who have been following the discussions on the “wetness” and the “normalized concentration” techniques: which of these two techniques is more fundamental?

The source solute could come in the form of gas, liquid or solid and could be absorbed into gas, liquid, or solid absorbents. However, all the publications on the use of the “wetness” technique for microelectronic assemblies so far have focused only on water vapor as the source solute and on solid absorbents [2,7–9]. This may have given the false impression that the technique is valid only for gaseous source solute and for solid absorbents.

The Henry's law, which suggests a linear sorption isotherm is valid only for dilute solutes [3,4]. The full range of sorption isotherms of solute-absorbents are typically non-linear [10]; for example the Langmuir's sorption isotherm is asymptotic [11]. Yoon et al. [12] have asserted that thermal-mass diffusion analogy is strictly for solute-absorbents that exhibit linear sorption isotherm; is this true?

It is known from experiments that the  $C_{sat}$  of an absorbent is dependent on the environmental temperature. A spatial variation in temperature could induce a spatial variation in  $C_{sat}$  even in a single-material absorbent and rendering the Fick's law inapplicable. The case of a temporal variation in temperature is more complicated; this would result in a temporal variation in  $C_{sat}$ , and hence a temporal discontinuity in “wetness”. The temporal discontinuity of “wetness” was first highlighted by Wong et al. [7]; while there have been methods proposed to address this issue [7,9,13,14], these are not entirely satisfactory either because of over-simplification or excessively complicated procedures.

The rest of the manuscript is organized into five sections; the correspondence between volumetric enthalpy and volumetric concentration is established, and the property “fractional saturation” is induced as a correspondence with temperature in Section 2; using the principle of equality of chemical potential, the continuity of “fractional saturation” is established in Section 3; its validity for non-linear sorption isotherm and its applicability to source solute and absorbents of diverse phases are also established in the same section, wherein, it is also shown that the “normalized concentration” is indeed a derived property of “wetness”; the techniques for

modeling absorbent with spatially varying temperature, source solute with time-varying concentration, and absorbent with multiple phases are discussed in Section 4; the complex problem of time-varying temperature is discussed in details in Section 5; this is followed by conclusions in Section 6.

## 2. The thermal-mass correspondences

### 2.1. Thermal diffusion

Fourier [15] in 1822 proposed the now well-known Fourier's law:

$$\mathbf{J}_q = -k_q \nabla T \quad (7)$$

where  $\mathbf{J}_q$  ( $\text{J s}^{-1} \text{m}^{-2}$ ) is heat flux and  $k_q$  ( $\text{J s}^{-1} \text{m}^{-1} \text{K}^{-1}$ ) is thermal conductivity, which suggests a linear relation between heat flux and the spatial gradient of temperature. Fourier's law as a fundamental law was affirmed by the zeroth law of thermodynamics, which states the continuity of temperature at the interface of substances, independent of the chemical constituents, the molecular/atomic structure, and the phases of the substances.

Under the condition of constant pressure, the first law of thermodynamics gives

$$dH_v = dq = \rho c_p dT \quad (8)$$

where  $H_v$  ( $\text{J m}^{-3}$ ) is the volumetric enthalpy,  $q$  ( $\text{J m}^{-3}$ ) the heat flow,  $\rho$  ( $\text{kg m}^{-3}$ ) the density, and  $c_p$  ( $\text{J kg}^{-1} \text{K}^{-1}$ ) the specific heat capacity at constant pressure. The multiplier  $\rho c_p$  ( $\text{J m}^{-3} \text{K}^{-1}$ ) is the volumetric heat capacity at constant pressure. Multiplying the right-hand side of Eq. (7) by  $\rho c_p / \rho c_p$  and assuming  $\rho c_p$  to be spatial-invariant gives

$$\mathbf{J}_q = -\alpha \nabla H_v \quad (9)$$

where  $\alpha = k_q / \rho c_p$  ( $\text{m}^2 \text{s}^{-1}$ ) is thermal diffusivity. Eq. (9) suggests a linear relation between heat flux and the spatial gradient of volumetric enthalpy, which appears to be the exact equivalence of the Fourier's law. Fig. 1 shows two substances that are in physical contact. The volumetric heat capacity of the two substances are such that  $(\rho c_p)_B > (\rho c_p)_A$ ; thus, a discontinuity in the volumetric enthalpy  $H_{v,A} = (\rho c_p)_A T$  and  $H_{v,B} = (\rho c_p)_B T$  develops at the interface of the two substances. Therefore, unlike Eq. (7), Eq. (9) is not a fundamental equation but it is valid only for a body that has a spatially uniform volumetric heat capacity ( $\rho c_p$ ).

Substituting Eq. (7) into the equation of conservation of heat energy (at constant pressure),

$$\frac{\partial H_v}{\partial t} + \nabla \cdot \mathbf{J}_q = \Theta_q \quad (10)$$

where  $\Theta_q$  ( $\text{J m}^{-3} \text{s}^{-1}$ ) is the internal heat source, and assuming  $\rho c_p$  to be time-invariant and  $k_q$  to be spatial-invariant, gives the heat diffusion equation:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{\Theta_q}{\rho c_p} \quad (11)$$

It is worth highlighting that the assumptions that have led to the above heat diffusion equation in its simplest form are intended to

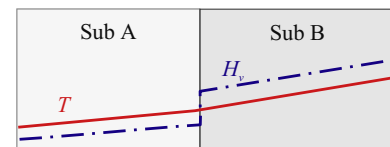


Fig. 1. The profiles of temperature and volumetric enthalpy in a body of two contacting substances.

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