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Assessment of steady state diffusion of volatile organic compounds in unsaturated building materials based on fractal diffusion model

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ABSTRACT

This paper presents a preliminary work to evaluate the steady state diffusion of volatile organic compounds (VOCs) in unsaturated building materials based on a newly-proposed fractal diffusion model. This model studies the contributions of water and gas to the diffusion transportation in unsaturated building materials, involves geometry parameters of unsaturated building materials, fractal dimensions, minimal and maximal pore diameters. In this model, the derivation of some parameters is assisted by newly-established three phases fractal carpet consisting of middle and peripheral parts that represent gas and water occupied regions in the unsaturated building materials. The influences of some structural parameters (removed number, recursion number and size) of fractal carpet on diffusion performance have been discussed. Additionally, the effective diffusion coefficients of various kinds of volatile organic compounds (formaldehyde, methanol, 1,3,5-trimethylbenzene, Ethylbenzene, xylene isomers, benzene and toluene) are also compared based on this fractal model. Formaldehyde exhibits the largest value of effective diffusion coefficient among selected VOCs.

1. Introduction

Building materials are the most used artificial materials in the world, and more than 2.5 tons of building materials are consumed per person yearly [1]. Normally, volatile organic compounds (VOCs) produced from many building materials have vapor pressures greater than 0.1 mm of Hg at standard condition (20 °C and 760 mm Hg) and are considered as the major sources resulting in poor indoor air quality, which is potentially dangerous to the health of human being [2–5]. One of the challenges in the utilization of building materials is to avoid the excessive emission of VOCs in indoor environment [3,4].

From the view point of experimental technique, environmental chambers testing approaches are commonly employed to detect the emission of VOCs from building materials [6–8]. However, questions regarding the performance of environmental chamber testing systems and the errors associated with the measurements of VOCs from building materials have been raised: results measured from environmental chamber testing systems present considerably scattered distribution [9], as shown in Table 1. This may be attributed to two factors [7]: 1) the reliable diffusion values of building materials are still unknown until now, it is thus lack of critical value for comparing the results among various laboratory measurements; and 2) different building materials/VOCs/test methods/conditions used in various laboratories may be one of sources of scattered data [10–18]. In particular, some studies considered that either chamber testing approaches or other cup methods may be inappropriate for some porous materials [14,17]. On the other hand, theoretically, several researchers have attempted to model the diffusion-driven emission of VOCs based on fluid dynamics in completely dry or wet building materials [6,19,20]. Shen et al. and Crawford et al. extended the classical Fick's diffusion law to a fractal diffusion model of VOCs in dry porous building materials [19,21]. Altinkaya, Chang et al. and Li et al., improved the classical vapor pressure and boundary layer model by considering the mass transfer process inside the wet materials [6,20,22,23]. However, in practices, most of building materials in nature usually exhibit unsaturated feature [24], viz., are partially full of water or gas. Therefore, there are still some limitations to applying these developed models to unsaturated building materials.

Besides, Winslow found that the surface of hydrated building materials presented typical fractal characteristic based on X-ray scattering technique [25]. Diamond and Bonen interpreted pore system of building materials using a fractal concept [26]: the

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Table 1
Comparison of effective diffusion coefficients of building materials from previous literatures.

Materials	Compound	Test method/condition	Effective diffusion coefficients (m^2/s)
Conventional gypsum wallboard [17]	Formaldehyde (CH_2O)	A dynamic dual-chamber, 50% RH	6.34×10^{-8}
"Green" gypsum wallboard [17]	Formaldehyde (CH_2O)	A dynamic dual-chamber, 50% RH	2.24×10^{-8}
Calcium silicate [16]	Formaldehyde (CH_2O)	A dynamic dual-chamber, 50%RH	3.28×10^{-6}
Medium density fireboard [15]	Formaldehyde (CH_2O)	C-history method in closed chamber,50%RH	8.15×10^{-8}
Painted drywall [11]	Ethylbenzene ($C_6H_5\ CH_2CH_3$)	Environmental chamber,50%RH	2.68×10^{-8}
Cement slab [12]	Ethylbenzene ($C_6H_5\ CH_2CH_3$)	Field and laboratory emission cell,25°	1.72×10^{-10}
Cement slab [12]	p-Xylene ($C_6H_4(CH_3)_2$)	Field and laboratory emission cell,25°	1.77×10^{-10}
Cement slab [12]	Toluene ($C_6H_5CH_3$)	Field and laboratory emission cell,25°	1.47×10^{-10}
Saturated inactive clay [10]	Benzene (C_6H_6)	A double-reservoir glass diffusion cell test	$(1.5–5.0) \times 10^{-10}$

relationship between fractal feature of microstructure and earlier classifications of building materials has been discussed. Lange et al. provided a comprehensive insight into the nature of fractal pore structure of building materials observed from massive backscattered electron images [27]. Livingston described the nucleation and growth for the hydration of main raw building materials based on a fractal model [28]. Arandigoyen and Alvarez investigated microstructure development of building materials taking into account porosity, pore size distribution and surface fractal dimension [29]. In the meantime, recent studies show plentiful of relations enabling the effective evaluation of physical quantities, such as permeability of fluids or heat transportation in porous building materials [30,31], to the representation of fractal geometry based on two-dimensional Sierpinski carpet or three-dimensional Menger sponge [32,33]. Therefore, it is possible to develop a rational fractal model to evaluate the diffusion performance of VOCs based on pore transportation mechanism in unsaturated building materials.

In particular, intrinsic pore structure parameters (porosity, pore size distribution and pore tortuosity) of building materials play an important role in gas/ion/VOCs diffusion performance [34]. Generally, pore structure may evolve with hydration or service time [34]. For an example, the commonly-used building materials, namely, cement-based materials usually have lower porosity, more tortuous pore paths and small pores as the hydration or service time increases [34–36]. Therefore, the well-understanding of VOCs diffusion performance in building materials is extremely significant to improve the indoor air quality of building environment.

In this work, the unsaturated building materials are referred to as the ones with time-dependent pore structure. A fractal diffusion model for unsaturated building materials based on pore transportation mechanism is established when the effects of diffusion of gas and water are considered. Some key parameters involved in this fractal model are obtained from the construction of three phases fractal carpet. The influences of structural parameters of fractal carpet and various kinds of VOCs on diffusion transportation performance in unsaturated building materials are evaluated.

2. Fractal diffusion model for unsaturated building materials

According to the fractal feature of porous media, the amount of pores, δN_w and δN_g, within pore diameter d and $(d + \delta d)$ for water saturated and gas pore channels are expressed as [37]:

$$\delta N_w = -D_{fw} d_{\max,w}^{D_{fw}} d^{-1-D_{fw}} \delta d \tag{1}$$

$$\delta N_g = -D_{fg} d_{\max,g}^{D_{fg}} d^{-1-D_{fg}} \delta d \tag{2}$$

where D_{fw}, D_{fg}, $d_{\max,w}$ and $d_{\max,g}$ are fractal dimensions for pore space and maximal pore diameters for water saturated and gas pore channels.

With respect to unsaturated building materials, the flow rates for water saturated and gas pore channels,$q_w(d)$ and $q_g(d)$, through a particular single tortuous path are given [31]:

$$q_w(d) = D_w \Delta c A_w(d)/L_w(d) = D_w \Delta c \pi d^2 \Big/ \left(4 d^{1-D_{tw}} L_0^{D_{tw}}\right) \tag{3}$$

$$q_g(d) = D_g \Delta c A_g(d)/L_g(d) = D_g \Delta c \pi d^2 \Big/ \left(4 d^{1-D_{tg}} L_0^{D_{tg}}\right) \tag{4}$$

where D_w and D_g are molecular diffusion coefficients of investigated VOCs in water and air, respectively; Δc is the concentration gradient between two ends of pore channels; L_0 is the length of building materials; D_{tw},D_{tg},$A_w(d)$,$A_g(d)$,$L_w(d)$ and $L_g(d)$ are fractal dimensions associated with pore tortuosity, cross sectional areas with diameter d and actual lengths of channels which are satisfied with typical fractal law for water saturated and gas pore channels [31].

The mass flow rate for water saturated and gas pore channels, Q_w and Q_g, can be obtained further by integrating individual flow rate over the corresponding pore ranges [37]:

$$Q_w = -\int_{d_{\min,w}}^{d_{\max,w}} q_w(d) \delta N_w = \frac{\pi D_w \Delta c D_{fw} d_{\max,w}^{D_{fw}}}{4 L_0^{D_{tw}} \left(D_{tw} - D_{fw} + 1\right)} \left(d_{\max,w}^{D_{tw}-D_{fw}+1} - d_{\min,w}^{D_{tw}-D_{fw}+1}\right) \tag{5}$$

$$Q_g = -\int_{d_{\min,g}}^{d_{\max,g}} q_g(d) \delta N_g = \frac{\pi D_g \Delta c D_{fg} d_{\max,g}^{D_{fg}}}{4 L_0^{D_{tg}} \left(D_{tg} - D_{fg} + 1\right)} \left(d_{\max,g}^{D_{tg}-D_{fg}+1} - d_{\min,g}^{D_{tg}-D_{fg}+1}\right) \tag{6}$$

where $d_{\min,w}$ and $d_{\min,g}$ are minimal pore diameters in water saturated and gas pore channels.

The total flow rate (Q_t) of VOCs through unsaturated building materials is derived as [38]:

$$Q_t = Q_w + Q_g \tag{7}$$

Some geometry parameters of unsaturated building materials can be established from pore structure information as [37]: