Available online at www.sciencedirect.com
ScienceDirect
International Journal of Heat and Mass Transfer 50 (2007) 2069–2077
International Journal of HEAT and MASS TRANSFER
www.elsevier.com/locate/ijhmt

An analytical mass transfer model for predicting VOC emissions from multi-layered building materials with convective surfaces on both sides

H.P. Hu [a], Y.P. Zhang [b,*], X.K. Wang [b], J.C. Little [c]

[a] Department of Thermal Science and Energy Engineering, University of Science and Technology of China, Hefei, 230026, PR China
[b] Department of Building Science, Tsinghua University, Beijing, 100084, PR China
[c] Department of Civil and Environmental Engineering, Virginia Tech, Blacksburg, VA 24060, United States

Received 6 September 2005; received in revised form 10 September 2006
Available online 17 January 2007

Abstract

An analytical mass transfer model for predicting emissions of Volatile Organic Compounds (VOCs) from multi-layered building materials and the instantaneous VOC material-phase distribution is developed. Different from the mass transfer models in the literature, it is able to describe the characteristics of VOC emissions from a wall with an arbitrary number of layers of different materials and with convective surfaces on both sides, and it does not neglect the mass transfer resistance through the gas-phase boundary layer. The model is validated with experimental data from the literature. The model provides a powerful tool for predicting VOC emissions from composite materials such as furniture and layered wall structures. Based upon the model and the dimensionless analysis, the applicable condition of Kumar and Little's double-layer model is discussed.

Keywords: VOC; Mass transfer; Indoor air quality; Modeling; Building material

1. Introduction

Indoor air quality is receiving increasing attention because most people spend most of their time indoors. In many buildings, the emissions of VOCs from building materials and furniture may reduce indoor air quality which may cause general symptoms, such as headache; eye, nose, or throat irritations; dry cough; dizziness and nausea; difficulty in concentrating; tiredness [1–3]. VOC emission from building materials is an important issue for many building designers and is included in regulations in both USA and Europe [4]. Therefore, accurate modeling of the material emission rate in a building is important for predicting the indoor contaminant concentration, occupant exposure, and for the design of the mechanical ventilation system.

Published approaches to studying the characteristics of VOC sources and sinks fall into two categories: experimental investigation, and modeling and simulation [5–28]. While experimental methods provide realistic results, they require expensive, full-scale and well-controlled facilities. Furthermore, the results obtained under the test condition may not be directly applicable to other conditions [29] and do not give insight into the physical mechanism governing emissions. As a result, many researchers have addressed the topic of modeling emissions of VOCs from building materials and furnishings in ventilated space.

Generally speaking, there are two kinds of VOC emission models in the literature [13,30]. The first kind is the so-called empirical or semi-empirical model. The parameters of empirical models are determined by fitting experimental data to the predefined model. Although an

* Corresponding author. Tel.: +86 10 6277 2518; fax: +86 10 6277 3461.
E-mail address: zhangyp@mail.tsinghua.edu.cn (Y.P. Zhang).

0017-9310/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijheatmasstransfer.2006.11.024

Nomenclature

A	emission area of building material
Bi_m	mass transfer Biot number
C_i	concentration of compound in the ith layer of building material (mg m^{-3})
$C_{0,i}(x)$	initial concentration of compound in the ith layer of building material (mg m^{-3})
$C^*_{0,i}$	dimensionless initial VOC concentration in material
$C_{i,s}(t)$	concentration of compound in the air adjacent to the interface (mg m^{-3}) $(i = 0, N+1)$
$C_{i,\infty}(t)$	concentration of compound in atmosphere or in chamber (mg m^{-3}) $(i = 0, N+1)$
C^*	dimensionless VOC concentration in material
D_i	mass diffusion coefficient for compound in the ith layer of building material
D^*_i	dimensionless diffusion coefficient in double-layer building material
Fo_m	mass transfer Fourier number
$h_{m,i}$	convective mass transfer coefficient $(i = 0, N+1)$
K_i	partition coefficient of the ith layer of building material
K^*_i	dimensionless partition coefficient
$\dot{m}_i(t)$	emission rate per unit area of VOC from the ith emission surface at time t (mg m^{-2} s^{-1}) $(i = 0, N+1)$
Q_i	volumetric air flow rate through the chamber in contact with the ith layer of double material $(i = 0, N+1)$
R^*	dimensionless VOC emission rate
t	time
V_i	volume of air in the chamber in contact with the ith layer of double material (m^{-3}) $(i = 0, N+1)$
x	linear distance (m)
X	dimensionless coordinate in mass transfer direction

Subscript

i	the layer's number identification, $(i = 1, 2, \ldots, N)$

Superscript

*	dimensionless parameter

empirical model is simple and easy to use, it is generally unable to provide any mechanistic insight. Also, it is difficult to scale the results from the chamber to building conditions. The second type is based on mass transfer theory and is referred to as a mass-transfer or physically-based model [5,9,12,30–33]. In contrast to empirical models, validated mass-transfer models can predict VOC emission for a wide range of conditions using known physical parameters. All the mass transfer models published before 2003, such as those developed by Clausen et al. [6], Dunn [9] and Little et al. [12], neglect the mass transfer resistance through the air phase boundary layer, and assumed that the initial VOC concentration distribution is uniform throughout the building material. Although this may be suitable for some building materials, the assumption as a general one has not been well verified [34], and may cause some obvious errors under certain conditions [31,32]. Huang and Haghighat [35] considered the mass transfer resistance through the air phase boundary layer, but assumed that the VOC concentration in ambient air, C_∞, is zero to obtain an analytical solution. Obviously, this assumption is not generally applicable. Besides, the convective mass transfer coefficient in Huang's model was estimated by the classical correlation for a flat plate, which is not necessarily correct for the chamber flow conditions. That was also a limitation of Huang's model. Recently, several papers extended the aforementioned works and obtained analytical solutions. The main extensions are as follows: (1) the initial contaminant concentration is not necessarily uniformly distributed [32,36]; (2) the mass transfer resistance through the air phase boundary layer is not neglected [31,37]; (3) the building material can be double-layer with one emission surface [38]; (4) the building material can be single layer with double emission surfaces [39]. Besides those papers, Zhang and Niu [40] numerically studied the characteristics of multi-layered building material with a single emission surface. All of the aforementioned models solve problems of building material VOC emissions. Contrary to this, Niu and co-workers developed some inverse models to determine D, K and C_0 from emission data for single layer building materials [27,28,41]. Up to now, however, no general analytical model for predicting emissions from multi-layered building materials has been reported in the literature. The objective of this paper is to develop a general mass-transfer model for analyzing double surface VOC emissions from arbitrary layered building materials in which the mass transfer resistance through the gas-phase boundary layer is not neglected and the initial distribution of material-phase VOC concentration in each layer of building material is not necessarily uniform.

2. Development of model

The model is developed based on the following assumptions: (1) all physical properties including diffusion coefficient and material/air partition coefficient for each layer are constant; (2) mass transfer through the material is

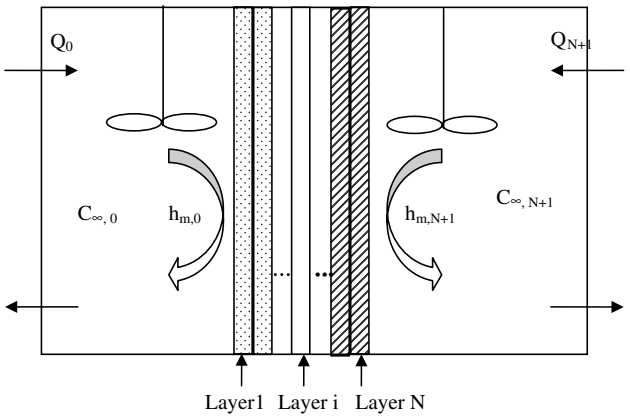

Fig. 1. Schematic of a multi-layered building material in contact with air.

one-dimensional; (3) the convective mass transfer coefficients are constant; (4) the gas phase VOC concentrations adjacent to both material surfaces are uniform although they may be different; (5) there is neither VOC source nor sink in the material. The problem is schematically shown in Fig. 1. The governing equations describing the transient mass diffusion through the material are:

$$D_i\frac{\partial^2 C_i}{\partial x^2}=\frac{\partial C_i}{\partial t},\quad t>0,\quad l_{i-1}<x<l_i,\quad i=1,2,\ldots N \tag{1}$$

The boundary conditions are:

$$D_1\frac{\partial C_1}{\partial x}=h_{\mathrm{m},0}(C_{0,s}(t)-C_{0,\infty}(t)),\quad t>0,\ x=l_0=0, \tag{2a}$$

$$C_1=K_1C_{0,s}(t),\quad t>0,\ x=l_0=0; \tag{2b}$$

$$D_i\frac{\partial C_i}{\partial x}=D_{i+1}\frac{\partial C_{i+1}}{\partial x},\quad t>0,\ x=l_i,\ i=1,2,\ldots N-1, \tag{3a}$$

$$\frac{C_i}{K_i}=\frac{C_{i+1}}{K_{i+1}},\quad t>0,\ x=l_i,\ i=1,2,\ldots N-1; \tag{3b}$$

$$-D_N\frac{\partial C_N}{\partial x}=h_{\mathrm{m},N+1}(C_{N+1,s}(t)-C_{N+1,\infty}(t)),\quad t>0,\ x=l_N, \tag{4a}$$

$$C_N=K_NC_{N+1,s}(t),\quad t>0,\ x=l_N; \tag{4b}$$

The initial condition is:

$$C_{0,i}(x)=f_i(x),\quad t=0,\quad l_{i-1}\leqslant x\leqslant l_i,\quad i=1,2,\ldots N. \tag{5}$$

The solution to Eqs. (1)–(5) derived by us is:

$$\begin{aligned}C_i(x,t)&=K_i[R_i(x)C_{0,\infty}(t)+(1-R_i(x))C_{N+1,\infty}(t)]\\&+\sum_{n=1}^{\infty}\frac{K_i}{\beta_n^2N(\beta_n)}\Psi_i(\beta_n,x)\Big\{[\beta_n^2F(\beta_n)-(h_{m,0}\Psi_1(\beta_n,l_0)C_{0,\infty}(0)\\&+h_{m,N+1}\Psi_N(\beta_n,l_N)C_{N+1,\infty}(0))]\mathrm{e}^{-\beta_n^2t}\\&-\Big[\int_0^t\mathrm{e}^{-\beta_n^2(t-\tau)}h_{m,0}\Psi_1(\beta_n,l_0)\mathrm{d}C_{0,\infty}(\tau)\\&+\int_0^t\mathrm{e}^{-\beta_n^2(t-\tau)}h_{m,N+1}\Psi_N(\beta_n,l_N)\mathrm{d}C_{N+1,\infty}(\tau)\Big]\Big\},\\&(l_{i-1}<x<l_i,i=1,2,\ldots,N),\end{aligned} \tag{6}$$

where

$$\begin{aligned}R_i(x)&=\frac{h_{m,0}}{h_{m,0}+h_{m,0}h_{m,N+1}\sum_{j=1}^{N}\frac{l_j-l_{j-1}}{K_jD_j}+h_{m,N+1}}\\&\times\left(1+h_{m,N+1}\times\left(\frac{l_i-x}{K_iD_i}+\sum_{j=i+1}^{N}\frac{l_j-l_{j-1}}{K_jD_j}\right)\right),\\&(l_{i-1}<x<l_i,i=1,2,\ldots,N),\end{aligned} \tag{6-1}$$

$$\text{for}\quad i=1,\ \text{or}\ i=N,\quad \sum_{j=i+1}^{N}\frac{l_j-l_{j-1}}{K_jD_j}\equiv 0. \tag{6-2}$$

$$N(\beta_n)=\sum_{i=1}^{N}K_i\int_{l_{i-1}}^{l_i}[\Psi_i(\beta_n,x')]^2\mathrm{d}x' \tag{6-3}$$

$$F(\beta_n)=\sum_{i=1}^{N}\int_{l_{i-1}}^{l_i}\Psi_i(\beta_n,x')f_i(x')\mathrm{d}x' \tag{6-4}$$

$$\begin{aligned}&\Psi_i(\beta_n,x)=A_{i,n}\sin\left(\frac{\beta_n}{\sqrt{D_i}}x\right)+B_{i,n}\cos\left(\frac{\beta_n}{\sqrt{D_i}}x\right),\\&l_{i-1}<x<l_i,\quad i=1,2,\ldots N\end{aligned} \tag{6-5a}$$

$$\begin{bmatrix}A_{i,n}\\B_{i,n}\end{bmatrix}=\left(\prod_{j=1}^{i-1}U_{j+1}^{-1}(l_j)U_j(l_j)\right)\begin{bmatrix}\frac{h_{m,0}}{\beta_nK_1\sqrt{D_1}}\\1\end{bmatrix},\quad i=1,2,\ldots,N \tag{6-5b}$$

$$\text{where}\quad U_j(x)=\begin{bmatrix}\sin\left(\frac{\beta_n}{\sqrt{D_j}}x\right) & \cos\left(\frac{\beta_n}{\sqrt{D_j}}x\right)\\ K_j\sqrt{D_j}\cos\left(\frac{\beta_n}{\sqrt{D_j}}x\right) & -K_j\sqrt{D_j}\sin\left(\frac{\beta_n}{\sqrt{D_j}}x\right)\end{bmatrix},\quad j=1,2,\ldots,N \tag{6-5c}$$

$$\text{for}\quad i=1,\quad \prod_{j=1}^{i-1}U_{j+1}^{-1}(l_j)U_j(l_j)\equiv I_2=\begin{bmatrix}1&0\\0&1\end{bmatrix} \tag{6-5d}$$

$\beta_n (n = 1, 2, \ldots)$ are the roots of the following equation:

$$\begin{vmatrix} v_{1,1} & v_{1,2} & 0 & & & \cdots & & & \cdots & & & 0 \\ & & \ddots & & & & & & & & & \\ & & & \ddots & & & & & & & & \\ 0 & \cdots & \cdots & 0 & v_{2i,2i-1} & v_{2i,2i} & v_{2i,2i+1} & v_{2i,2i+2} & 0 & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & 0 & v_{2i+1,2i-1} & v_{2i+1,2i} & v_{2i+1,2i+1} & v_{2i+1,2i+2} & 0 & \cdots & \cdots & 0 \\ & & & & & & & & \ddots & & & \\ & & & & & & & & & \ddots & & \\ 0 & & & \cdots & & & \cdots & & & 0 & v_{2N,2N-1} & v_{2N,2N} \end{vmatrix} = 0 \tag{6-6}$$

$$v_{1,1} = -\beta_n K_1 \sqrt{D_1}, \quad v_{1,2} = h_{m,0};$$

$$v_{2i,2i-1} = \sin\left(\frac{\beta_n}{\sqrt{D_i}} l_i\right), \quad v_{2i,2i} = \cos\left(\frac{\beta_n}{\sqrt{D_i}} l_i\right),$$

$$v_{2i,2i+1} = -\sin\left(\frac{\beta_n}{\sqrt{D_{i+1}}} l_i\right), \quad v_{2i,2i+2} = -\cos\left(\frac{\beta_n}{\sqrt{D_{i+1}}} l_i\right),$$

$$v_{2i+1,2i-1} = K_i \sqrt{D_i} \cos\left(\frac{\beta_n}{\sqrt{D_i}} l_i\right),$$

$$v_{2i+1,2i} = -K_i \sqrt{D_i} \sin\left(\frac{\beta_n}{\sqrt{D_i}} l_i\right),$$

$$v_{2i+1,2i+1} = -K_{i+1} \sqrt{D_{i+1}} \cos\left(\frac{\beta_n}{\sqrt{D_{i+1}}} l_i\right),$$

$$v_{2i+1,2i+2} = K_{i+1} \sqrt{D_{i+1}} \sin\left(\frac{\beta_n}{\sqrt{D_{i+1}}} l_i\right);$$

$$(i = 1, 2, \ldots, N-1)$$

$$v_{2N,2N-1} = \beta_n K_N \sqrt{D_N} \cos\left(\frac{\beta_n}{\sqrt{D_N}} l_N\right) + h_{m,N+1} \sin\left(\frac{\beta_n}{\sqrt{D_N}} l_N\right),$$

$$v_{2N,2N} = -\beta_n K_N \sqrt{D_N} \sin\left(\frac{\beta_n}{\sqrt{D_N}} l_N\right) + h_{m,N+1} \cos\left(\frac{\beta_n}{\sqrt{D_N}} l_N\right).$$

$$\dot{m}_0(t) = -R(C_{0,\infty}(t) - C_{N+1,\infty}(t)) + \sum_{n=1}^{\infty} \frac{h_{m,0}}{\beta_n^2 N(\beta_n)} \left\{ [\beta_n^2 F(\beta_n) - (h_{m,0} C_{0,\infty}(0) + h_{m,N+1} \Psi_N(\beta_n, l_N) C_{N+1,\infty}(0))] e^{-\beta_n^2 t} - \left[\int_0^t e^{-\beta_n^2 (t-\tau)} h_{m,0} dC_{0,\infty}(\tau) + \int_0^t e^{-\beta_n^2 (t-\tau)} h_{m,N+1} \Psi_N(\beta_n, l_N) dC_{N+1,\infty}(\tau) \right] \right\} \tag{7}$$

where

$$R = \frac{h_{m,0} h_{m,N+1}}{h_{m,0} + h_{m,0} h_{m,N+1} \sum_{j=1}^{N} \frac{l_j - l_{j-1}}{K_j D_j} + h_{m,N+1}} \tag{7-1}$$

$$\dot{m}_{N+1}(t) = R(C_{0,\infty}(t) - C_{N+1,\infty}(t)) + \sum_{n=1}^{\infty} \frac{h_{m,N+1}}{\beta_n^2 N(\beta_n)} \Psi_N(\beta_n, l_N) \times \left\{ \left[\beta_n^2 F(\beta_n) - (h_{m,0} C_{0,\infty}(0) + h_{m,N+1} \Psi_N(\beta_n, l_N) C_{N+1,\infty}(0) \right] e^{-\beta_m^2 t} - \left[\int_0^t e^{-\beta_n^2 (t-\tau)} h_{m,0} dC_{0,\infty}(\tau) + \int_0^t e^{-\beta_n^2 (t-\tau)} h_{m,N+1} \Psi_N(\beta_n, l_N) dC_{N+1,\infty}(\tau) \right] \right\}. \tag{8}$$

To obtain the indoor VOC concentration, the following equation is needed to combine Eqs. (7) and (8):

$$V_i \frac{dC_{i,\infty}}{dt} = A_i \dot{m}_i(t) - Q_i C_{i,\infty}, \quad i = 0 \text{ or } N+1. \tag{9}$$

3. Validation of the model

3.1. Validation with experiment data from the literature

In Ref. [40], there is a validating experiment for multi-layered building material emission whose arrangement is shown in Fig. 2. The purified and humidity controlled air passed through a FLEC, a standard emission test chamber, where a double-layer material emitting VOCs was placed and the instantaneous concentrations of TVOC in the outlet of the FLEC were measured by GC/MS. The detailed fluid flow and mass transfer in the FLEC was studied by Zhang and Niu [42]. The parameters used by Zhang and Niu [40] for each layer of the material, and the parameters of the chamber and air flow conditions are shown in Table 1. Fig. 3 illustrates the chamber TVOC concentration simulated by the present model under the same condition as the experiment of Zhang and Niu. The model fits the experimental data well during the first 2 h although it slightly overestimates the chamber TVOC concentration

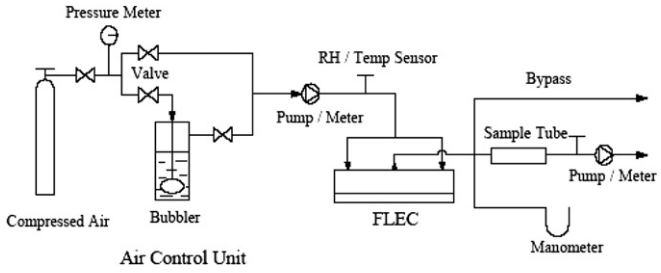

Fig. 2. Set up of emission test with a FLEC in Ref. [40].

Table 1
Experimental parameters in Ref. [40]

Volume of chamber (m^3)	3.5×10^{-5}
Air changer rate (h^{-1})	837
Area of the test material (m^2)	0.0177
The thickness of the top layer (m)	0.0008
The thickness of the bottom layer (m)	0.002
The mass diffusion coefficient of TVOC in the top layer (m^2/s)	1.04×10^{-12}
The mass diffusion coefficient of TVOC in the bottom layer (m^2/s)	1.00×10^{-14}
The partition coefficient of TVOC in the top layer (dimensionless)	40 560
The partition coefficient of TVOC in the bottom layer (dimensionless)	0.01
The initial material TVOC concentration in the top layer (mg/m^3)	248
The initial material TVOC concentration in the bottom layer (mg/m^3)	0
The convective mass transfer coefficient (m/s)	0.002

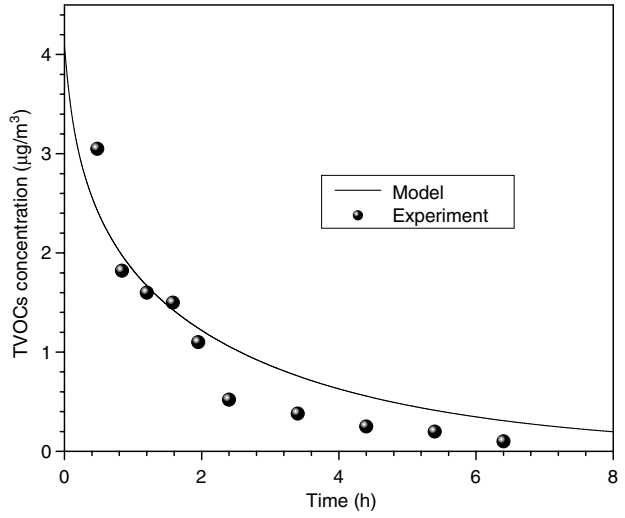

Fig. 3. Comparison of multi-layer model with experimental data in Ref. [40].

in the longer term. According to ASTM standard D 5157-97 (2003) [43], the correlation coefficient between experimental data and predicted data is also calculated as 0.972, which quantitatively certifies a good agreement.

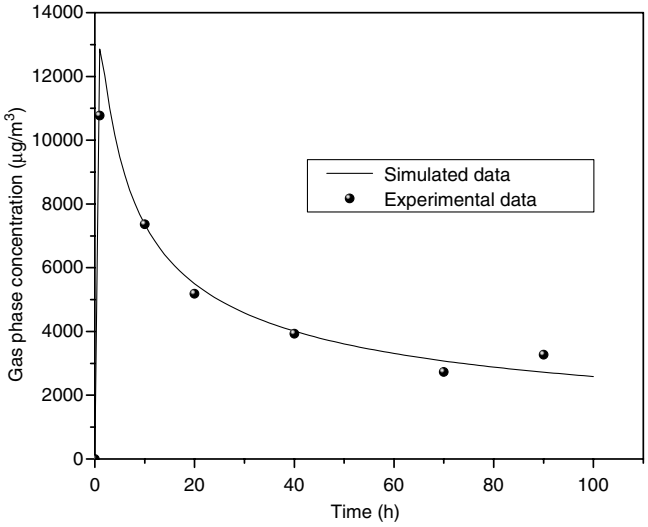

Fig. 4. Comparison with the experimental data in Ref. [44].

Table 2
Parameter list for the experiment described in Ref. [44]

Volume of chamber (m^3)	$0.5 \times 0.4 \times 0.25$
Air changer rate (h^{-1})	1.0 ± 0.05
Area of the test material (m^2)	0.212×0.212
The thickness of the material (m)	0.0159
The mass diffusion coefficient of TVOC in building material (m^2/s)	7.65×10^{-11}
The partition coefficient of TVOC in material (dimensionless)	3289
The initial material TVOC concentration in the material ($\mu g/m^3$)	9.86×10^7
The convective mass transfer coefficient (m/s)	0.00117

3.2. Self-examination

If the corresponding parameters of both layers in a double-layer material are the same, that is, $K_1 = K_2$, $D_1 = D_2$, and $C_{0,1} = C_{0,2}$, the double-layer material is equivalent to a single-layer material, so the proposed model can be validated with experimental results for single layer materials.

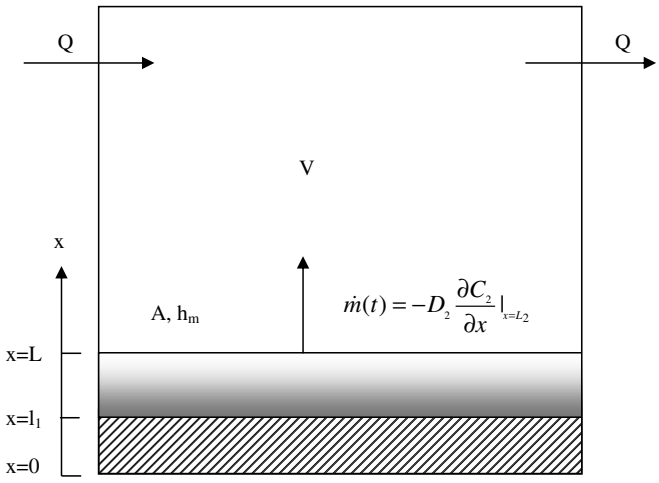

Fig. 5. Schematic of double layer building material in chamber.

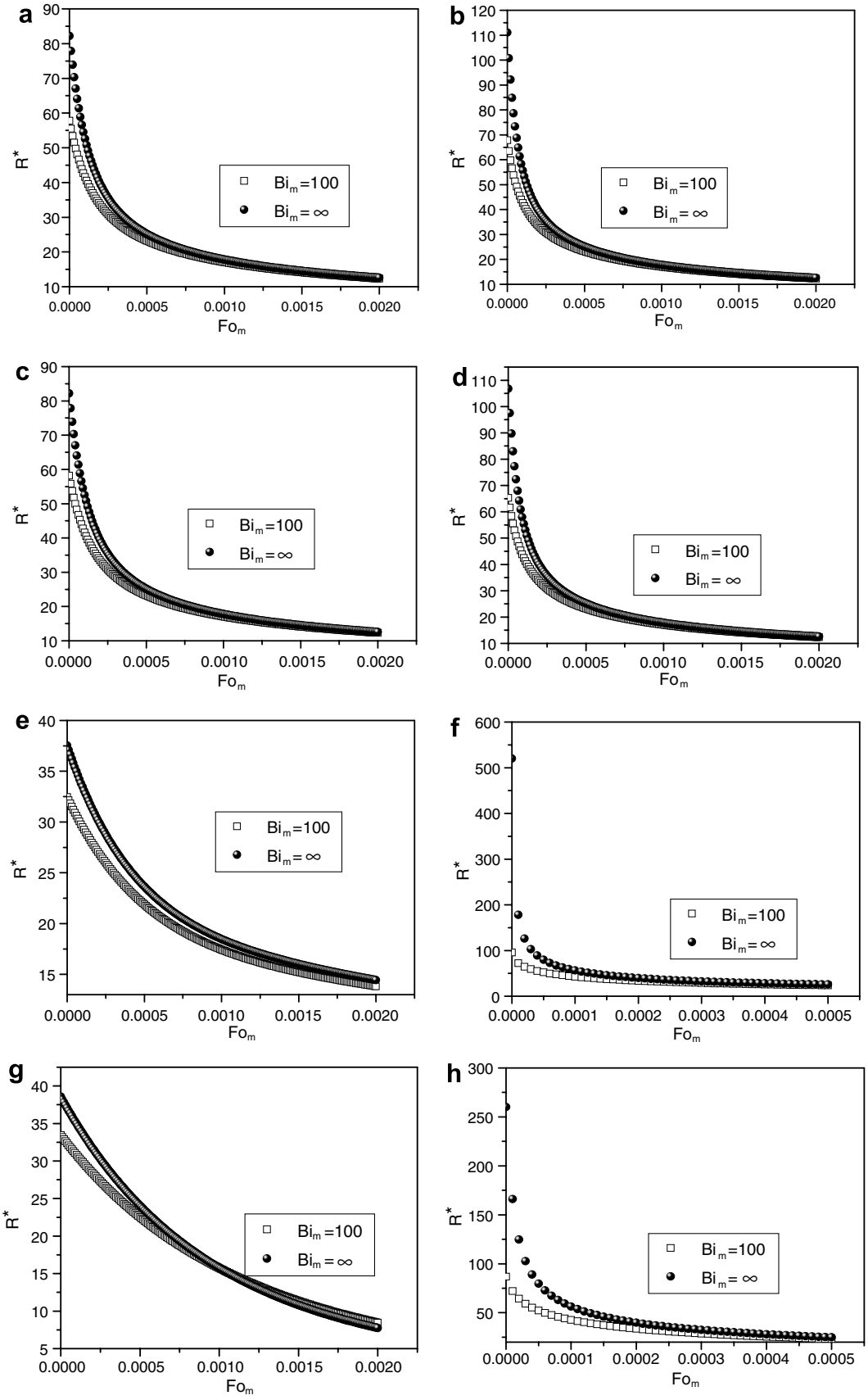

Fig. 6. Comparison of VOC emissions between $Bi_m = 100$ and $Bi_m = \infty$ under conditions (a)–(h).

Fig. 4 shows the comparison of the simulated results with the experimental data in Ref. [44]. The parameters in the simulated case including chamber-related parameters, diffusion coefficient and partition coefficient determined by Yang, are listed in Table 2. The results are in good agreement with a calculated correlation coefficient 0.990, which validates the proposed model.

4. Discussion

The proposed model can be used to analyze the applicable condition of Kumar and Little's double-layer model which neglects the mass transfer resistance through the material-air boundary layer. To discuss the problem more generally, it is helpful that the double-layer model (Fig. 5) is normalized. The following dimensionless parameters are defined:

$$C_i^* = \frac{C_i - K_i C_\infty}{C_{2,0} - K_2 C_\infty} \tag{10-1}$$

$$D_i^* = \frac{D_i}{D_2} \tag{10-2}$$

$$K_i^* = \frac{K_i}{K_2} \tag{10-3}$$

$$Fo_\mathrm{m} = \frac{D_2 t}{L^2} \tag{10-4}$$

$$Bi_\mathrm{m} = \frac{h_\mathrm{m} L}{D_2 K_2} \tag{10-5}$$

$$X = \frac{x}{L} \tag{10-6}$$

where it is assumed that the dimensionless initial concentrations in each layer of the material are both equal to 1 and the room VOC concentration is constant. Then according the foregoing multi-layer model, the double-layer model's governing equations and boundary conditions can be written in dimensionless form as follows:

$$D_i^* \frac{\partial^2 C_i^*}{\partial X^2} = \frac{\partial C_i^*}{\partial Fo_\mathrm{m}},$$

$$Fo_\mathrm{m} > 0, \quad 0 \leqslant \frac{l_{i-1}}{L} \leqslant X \leqslant \frac{l_i}{L} \leqslant 1, \quad (i = 1, 2) \tag{11-1}$$

$$\frac{\partial C_1^*}{\partial X} = 0, \quad Fo_\mathrm{m} > 0, \quad X = 0 \tag{11-2}$$

$$D_1^* \frac{\partial C_1^*}{\partial X} = \frac{\partial C_2^*}{\partial X}, \quad Fo_\mathrm{m} > 0, \quad X = \frac{l_1}{L} \tag{11-3}$$

$$\frac{C_1^*}{K^*} = C_2^*, \quad Fo_\mathrm{m} > 0, \quad X = \frac{l_1}{L} \tag{11-4}$$

$$\frac{\partial C_2^*}{\partial X} = Bi_\mathrm{m} C_2^*, \quad Fo_\mathrm{m} > 0, \quad X = 1 \tag{11-5}$$

$$C_{i,0}^* = 1, \quad Fo_\mathrm{m} = 0, \quad i = 1, 2 \tag{11-6}$$

From Eqs. (11-1)–(11-6), the dimensionless emission rate R^* is the function of $D_1^*, K_1^*, Bi_\mathrm{m}, \frac{l_1}{L}, Fo_\mathrm{m}$, i.e., $R^* = f(D_1^*, K_1^*, Bi_\mathrm{m}, \frac{l_1}{L}, Fo_\mathrm{m})$. Based on that, the dimensionless emission rate is calculated and the error of ignoring the convective mass transfer coefficient (i.e., assuming that $Bi_\mathrm{m} = \infty$) is known.

Table 3
Dimensionless parameters under conditions (a)–(h)

Condition	a	b	c	d	e	f	g	h
D_1/D_2	0.1	10	0.1	10	0.1	10	0.1	10
K_1/K_2	0.1	0.1	10	10	0.1	0.1	10	10
l_1/L	0.1	0.1	0.1	0.1	0.9	0.9	0.9	0.9

Fig. 6 gives the results of comparison between the two cases where $Bi_\mathrm{m} = 100$ and $Bi_\mathrm{m} = \infty$ under different conditions with the various dimensionless parameters (see Table 3). In all figures, Fo_m varies from 0 to 0.002, except in Fig. 6(f) and (h) because the difference between the two cases where $Bi_\mathrm{m} = 100$ and $Bi_\mathrm{m} = \infty$ after $Fo_\mathrm{m} = 0.0005$ can be neglected.

As shown in Fig. 6, the error of neglecting the mass transfer resistance through the material-air interface decreases with increasing Fo_m, so Kumar and Little's model is accurate enough in predicting long-term emission behavior of building material.

Estimation of the model parameters including $D_i, K_i, C_{0,i}$ and $h_{\mathrm{m},i}$ is an important issue for predicting VOC emission from multi-layered building materials. Some researchers have proposed experimental methods to determine D, K, C_0 of single layer building materials [8,27,28,41,44–47]. Therefore, the parameters for each layer can be measured separately by those methods. h_m is often estimated by some mass transfer correlations. However, some correlations used in the literature are not very suitable for the chamber problem studied. In some specific cases, if there is no suitable h_m correlation, additional work would be needed.

5. Conclusions

The present analytical model is suitable to describe the characteristics of DOUBLE surface VOC emission from ARBITRARY layers of building material instead of single surface emission from one or two layers of building material, and it does not neglect the mass transfer resistance through the gas-phase boundary layer. Using the proposed model and dimensionless analysis, the applicable condition of Kumar and Little's double-layer model is discussed. It is found that the error is significant in the early stage of emission, although it is convenient and accurate to simulate long-term emissions for double layer materials. The new multi-layer model generalizes the preceding mass-transfer models [12,31,32,35–39,44] and has been validated with experimental data in the literature. The model provides a powerful tool to predict VOC emissions from composite material systems.

Acknowledgements

This work was sponsored by the National Natural Science Foundation of China (Grant No. 50478012 and 50436040).

References

[1] Y.M. Kim, S. Harrad, R.M. Harrison, Concentrations and sources of VOCs in urban domestic and public microenvironments, Environ. Sci. Technol. 35 (2001) 997–1004.

[2] R. Meininghaus, T. Salthammer, et al., Interaction of volatile organic compounds with indoor materials-a small-scale screening method, Atmos. Environ. 33 (1999) 2395–2401.

[3] L. Molhave, The sick buildings and other buildings with indoor climate problems, Environment 15 (1989) 65–74.

[4] Y. Chuck, G. Derrick, A review of the emission of VOCs from polymeric materials used in buildings, Build. Environ. 22 (1998) 357–374.

[5] J.C.S. Chang, Z. Guo, Modeling of the fast organic emissions from a wood-finishing product-floor wax, Atmos. Enviro. 26 (1992) 2365–2370.

[6] P.A. Clausen, P. Wolkoff, et al., Long-term emission of volatile organic compounds from waterborne paints-methods of comparison, Indoor Air 4 (1991) 562–576.

[7] A. Colombo, M. De Bortoli, Comparison of models used to estimate parameters of organic emissions from materials tested in small environmental chambers, Indoor Air 2 (1992) 49–57.

[8] S.S. Cox, D. Zhao, J.C. Little, Measuring partition and diffusion coefficients for volatile organic compounds in vinyl flooring, Atmos. Environ. 35 (2001) 709–714.

[9] J.E. Dunn, Models and statistical methods for gaseous emission testing of finite source in well-mixed chambers, Atmos. Environ. 21 (1987) 425–430.

[10] J.E. Dunn, B.A. Tichenor, Compensating for sink effects in emissions test chambers by mathematical modeling, Atmos. Environ. 22 (1988) 885–894.

[11] F. Haghighat, Y. Zhang, Modeling of emission of volatile organic compounds from building materials-estimation of gas-phase mass transfer coefficient, Build. Environ. 34 (1999) 377–389.

[12] J.C. Little, A.T. Hodgson, A.J. Gadgil, Modeling emissions of volatile organic compounds from new carpets, Atmos. Environ. 28 (1994) 227–234.

[13] R. Merrill, R. Steiber, L. Nelms, Screening methods for the identification of organic emissions from indoor air pollution sources, Atmos. Environ. 21 (1987) 331–336.

[14] S. Murakami, S. Kato, et al., Distribution of chemical pollutants in a room based on CFD simulation coupled with emission/sorption analysis, ASHRAE Trans. 107 (2001) (pt. 1).

[15] S. Silberstein, R.A. Grot, I. Kunimichi, J.L. Mulligan, Validation of models for predicting formaldehyde concentrations in residences due to pressed-wood products, J. Air Pollut. Control Ass. 38 (1988) 1403–1411.

[16] L.E. Sparks, B.A. Tichenor, J.S. Chang, Z. Guo, Gas-phase mass transfer model for predicting volatile organic compound (VOC) emission rates from indoor pollutant sources, Indoor Air 6 (1996) 31–40.

[17] B.A. Tichenor, Z. Guo, J.E. Dunn, L.E. Sparks, M.A. Mason, The interaction of vapor phase organic compounds with indoor sink, Indoor Air 1 (1991) 23–25.

[18] B.A. Tichenor, Z. Guo, The effect of ventilation on emission rates of wood furnishing materials, Environ. Int. 17 (1991) 317–323.

[19] B.A. Tichenor, Z. Guo, L.E. Sparks, Fundamental mass transfer model for indoor air emission from surface coatings, Indoor Air 3 (1993) 263–268.

[20] C. Topp, P.V. Nielsen, P. Heiselberg, Influence of local air flow on the pollutant emission from indoor building surfaces, Indoor Air 11 (2001) 162–170.

[21] P. Wolkoff, P.A. Clausen, Application of fields and laboratory emission cell (FLEC) recovery study, case study of damaged linoleum, and liquid wax, Indoor Air 3 (1993) 543–549.

[22] X. Yang, Q. Chen, A coupled air flow and source/sink model for simulating indoor VOC exposures, Indoor Air 11 (2001) 257–269.

[23] D.Y. Zhao, J.C. Little, A.T. Hodgson, Modeling the reversible diffusive sink effect in response to transient contaminant sources, Indoor Air 12 (2002) 184–190.

[24] J.P. Zhu, J.S. Zhang, C.Y. Shaw, Comparison of models for describing measured VOC emissions from wood-based panels under dynamic chamber test condition, Chemosphere 44 (2001) 1253–1257.

[25] C.S. Lee, F. Haghighat, W.S. Ghaly, A study on VOC source and sink behavior in porous building materials-analytical model development and assessment, Indoor Air 15 (2005) 183–196.

[26] H.Y. Huang, F. Haghighat, Building materials VOC emissions – a systematic parametric study, Build. Environ. 38 (2003) 995–1005.

[27] F. Li, J.L. Niu, An inverse approach for estimating the initial distribution of volatile organic compounds in dry building material, Atmos. Environ. 39 (2005) 1447–1455.

[28] F. Li, J.L. Niu, An inverse technique to determine volatile organic compounds diffusion and partition coefficients in dry building material, Heat Mass Transfer 9 (2005) 834–842.

[29] D. Won, D.M. Sander, C.Y. Shaw, R.L. Corsi, Validation of the surface sink model for sorptive interactions between VOCs and indoor materials, Atmos. Environ. 35 (2001) 4479–4488.

[30] Z. Guo, Review of indoor emission source models. Part 1: Overview, Environ. Pollut. 120 (2002) 533–549.

[31] Y. Xu, Y.P. Zhang, An improved mass transfer based model for analyzing VOC emissions from building materials, Atmos. Environ. 37 (2003) 2497–2505.

[32] Y. Xu, Y.P. Zhang, A general model for analyzing single surface VOC emission characteristics from building materials and its application, Atmos. Environ. 38 (2004) 113–119.

[33] Y.P. Zhang, Y. Xu, Characteristics and correlations of VOC emissions from building materials, Int. J. Heat Mass Transfer 46 (2003) 4877–4883.

[34] J.D. Spengler, Q. Chen, K.M. Dilwali, Indoor air quality factors in designing a healthy building, in: J.D. Spengler, J.M. Samet, J.F. McCarthy (Eds.), Chapter 5 of Indoor Air Quality Handbook, McGraw-Hill Companies, Inc., New York, USA, 2001.

[35] H. Huang, F. Haghighat, Modelling of volatile organic compounds emission from dry building materials, Build. Environ. 37 (2002) 1349–1360.

[36] D. Kumar, J.C. Little, Single-layer model to predict the source/sink behavior of diffusion-controlled building materials, Environ. Sci. Technol. 37 (2003) 3821–3827.

[37] B.Q. Deng, C.N. Kim, An analytical model for VOCs emission from dry building materials, Atmos. Environ. 38 (2004) 1173–1180.

[38] D. Kumar, J.C. Little, Characterizing of the source/sink behavior of double-layer building materials, Atmos. Environ. 37 (2003) 5529–5537.

[39] X.K. Wang, Y.P. Zhang, R.Y. Zhao, Study on characteristics of double surface VOC emissions from dry flat-plate building materials, Chin. Sci. Bull. 51 (2006) 2287–2293.

[40] L.Z. Zhang, J.L. Niu, Modeling VOCs emissions in a room with a single-zone multi-component multi-layer technique, Build. Environ. 39 (2004) 523–531.

[41] R. Luo, J.L. Niu, Determination of water vapor diffusion and partition coefficients in cement using one FLEC, Int. J. Heat Mass Transfer 47 (2004) 2061–2072.

[42] L.Z. Zhang, J.L. Niu, Laminar fluid flow and mass transfer in a standard field and laboratory emission cell (FLEC), Int. J. Heat Mass Transfer 46 (2002) 91–100.

[43] ASTM, D 5157-97 (2003), Standard Guide for Statistical Evaluation of Indoor Air Quality Models, American Society for Testing and Materials, Philadelphia, PA., 2003.

[44] X. Yang, Study of Building Materials Emissions and Indoor Air Quality, Ph.D. thesis of Massachusetts Institute of Technology, 1999.
[45] F. Haghighat, C.S. Lee, W.S. Ghaly, Measurement of diffusion coefficients of VOCs for building materials: review and development of a calculation procedure, Indoor Air 12 (2002) 81–91.
[46] S.S. Cox, A.T. Hodgson, J.C. Little, Measuring concentrations of volatile organic compounds in vinyl flooring, J. Air Waste Manage. Assoc. 51 (2001) 1195–1201.
[47] Chinese National Standard GB/T 17657-1999, Test methods of evaluating the properties of wood-based panels and surface decorated wood-based panels.