A new model for analyzing the influence of initial concentration in building materials on VOC emission characteristics

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ABSTRACT
A new generally applicable model for calculating the surface emissions of VOCs (volatile organic compounds) from the building materials and the VOC instantaneous distributions in the materials is developed. Different from the mass transfer based models in the literature, the new model does not neglect the mass transfer resistance through the air phase boundary layer and does not assume that the initial VOC concentration distribution C_0 in building materials is uniform. And this paper provides an exact analytical solution for this model. For the specific case that C_0 is uniform, the proposed model is validated with experimental data. By using different distribution of initial VOC concentration in building materials, the influence of initial VOC concentration on VOC emission characteristics is clarified.

KEYWORDS: Model, VOCs, Mass diffusion, Indoor air quality, Building material.

INTRODUCTION
Low indoor air quality problem due to the emissions of volatile organic compounds (VOCs) from building materials, furniture and equipment may cause general symptoms, such as headache; eye, nose, or throat irritations; dry cough; dizziness and nausea; difficulty in concentrating; tiredness (Kim and Harrad, 2001; Yang, 1999). Since building materials are important sources of VOCs in indoor environment, it is necessary to know their emission characteristics.

The available methods of studying the characteristics of VOC sources and sinks in the literature fall into two categories: experimental investigation, modeling and simulation. Generally speaking, there are two kinds of VOC emission models in the literature. The first type is the so-called empirical model. It bases solely on the observation and statistical analysis of emission data obtained from environment chamber testing. The typical examples are the first-order decay model and power-law decay model (Zhu et al., 2001). Although an empirical model is simple and easy to use, it is not able to provide insight into the physical emission mechanisms. And it is difficult to scale the results from the chamber to building conditions. The second type of models is based upon the mass transfer theory and is thus called mass-transfer-based model. Unlike the empirical models, mass-transfer-based models can predict the VOC emission for various conditions when the physical parameters are known. Representative mass-transfer-based models are those developed by Dunn et al. (1987), Clausen et al. (1991), and Little et al. (1994). In order to obtain an analytical solution, these models neglected the mass transfer resistance through the air phase boundary layer. As to the applicable range of the aforementioned assumption and the relative error caused by the assumption, until now it has not been well analyzed in the literature. Yang et al. (2001) developed a numerical model to simulate dry material emission processes. Although the numerical model considered both the boundary layer resistance and internal resistance, it is not very convenient to use because it is time-consuming.

The objective of the present research is to extend the work to a more generalized case where the mass transfer resistance through the air phase boundary layer is not reflected and the distribution of initial VOC concentration in building materials is not necessarily uniform. The new model developed is analytical in nature and by using it, the characteristics of VOC emissions from building materials can be clarified.

DEVELOPMENT OF MODEL

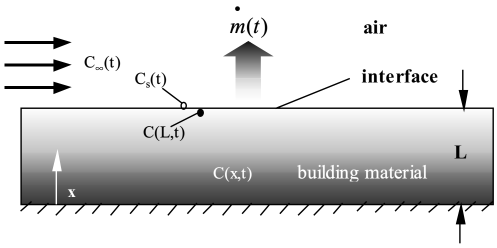


Fig.1 Schematic shown of a building material slab in atmosphere.

The model assumes that VOCs are emitted out of a single uniform layer of material slab with VOC-impermeable backing material, and a schematic of the idealized building material slab placed in atmosphere is shown in Fig.1. The governing equation describing the transient diffusion through the slab is

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2} \tag{1}$$

where C(x,t) is the concentration of the contaminant in the building material slab, t is time, and x is the linear distance. For given contaminant, the mass diffusion coefficient D is assumed to be constant. The initial condition assumes that the compound of interest is distributed throughout the building material slab as $C_0(x)$, or

$$C(x,0) = C_0(x) \quad \text{for} \quad 0 \le x \le L \tag{2}$$

where L is the thickness of the slab, and $C_0(x)$ is the distribution of initial contaminant concentration. It should be mentioned that almost all the physically based models in the literature assumed that $C_0(x)$ is uniformly, i.e., $C_0(x)=C_0$ (Little et al., 1994; X.Yang et al, 2001; Hongyu H, 2002). Obviously, the case assumed is a special case of equation (2). Since the slab is resting on a VOC-impermeable surface, the boundary condition of the lower surface of the slab is

$$\frac{\partial C(x,t)}{\partial t}=0, \qquad t>0, \quad x=0 \tag{3}$$

A third boundary condition is imposed on the upper surface of the slab (Fig.1)

$$-D\frac{\partial C(x,t)}{\partial x}=h_m(C_s(t)-C_\infty(t)), \qquad t>0, \quad x=L. \tag{4}$$

where h_m is the convective mass transfer coefficient, m/s; $C_s(t)$ is the concentration of VOC in the air adjacent to the interface; mg m^{-3}; $C_\infty(t)$ is the VOC concentration in atmosphere, mg m^{-3}. It should be mentioned that almost all the physically based models in the literature assumed $C_s(t)= C_\infty(t)$, i.e. implied that h_m is infinite, (Dunn, 1987; Clausen et al., 1991; Little et al., 1994). Obviously, the case assumed is a special case of equation (4). Besides, equilibrium exists between the contaminant concentrations in the surface layer of the slab and the ambient air, or (Little et al., 1994)

$$C(x,t)=KC_s(t), \qquad t>0, \quad x=L. \tag{5}$$

where K is the so-called partition coefficient.

The solutions to equations (1)-(5) derived by us are as follows

$$C(x,t)=KC_\infty(t)+\sum_{m=1}^{\infty}\frac{\sin(\beta_m L)}{\beta_m}\cdot\frac{2(\beta_m^2+H^2)}{L(\beta_m^2+H^2)+H}\cdot\cos(\beta_m x)\cdot \tag{6}$$

$$[(R_m-KC_\infty(0))e^{-D\beta_m^2 t}+\int_0^t e^{-D\beta_m^2(t-\tau)}\cdot KdC_\infty(\tau)]$$

where $H=\frac{h_m}{KD}$, $R_m=\frac{\beta_m}{sin(\beta_m L)}\int_0^L cos(\beta_m x')\cdot C_0(x')dx'$, β_m (m=1,2,…) are the positive

roots of $\beta_m\cdot tan(\beta_m L)=H$ (7)

Equation (6) gives the contaminant concentration in the building material slab as a function of distance from the base of the slab, and also of time.

Thus, VOC emission rate per unit area at instant t $\dot{m}(t)$ and VOC mass emitted from per unit area of the building material slab before instant t m(t) can be respectively expressed as follows

$$\dot{m}(t)=-D\cdot\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L}=D\cdot\sum_{m=1}^{\infty}\sin^2(\beta_m L)\cdot\frac{2(\beta_m^2+H^2)}{L(\beta_m^2+H^2)+H}\cdot$$

$$[(R_m-KC_\infty(0))e^{-D\beta_m^2 t}+\int_0^t e^{-D\beta_m^2(t-\tau)}\cdot KdC_\infty(\tau)] \tag{8}$$

$$m(t)=-\int_0^t D\cdot\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L}dt=D\int_0^t\sum_{m=1}^{\infty}\sin^2(\beta_m L)\cdot\frac{2(\beta_m^2+H^2)}{L(\beta_m^2+H^2)+H}\cdot$$

$$[(R_m-KC_\infty(0))e^{-D\beta_m^2 t}+\int_0^t e^{-D\beta_m^2(t-\tau)}\cdot KdC_\infty(\tau)]\ dt \tag{9}$$

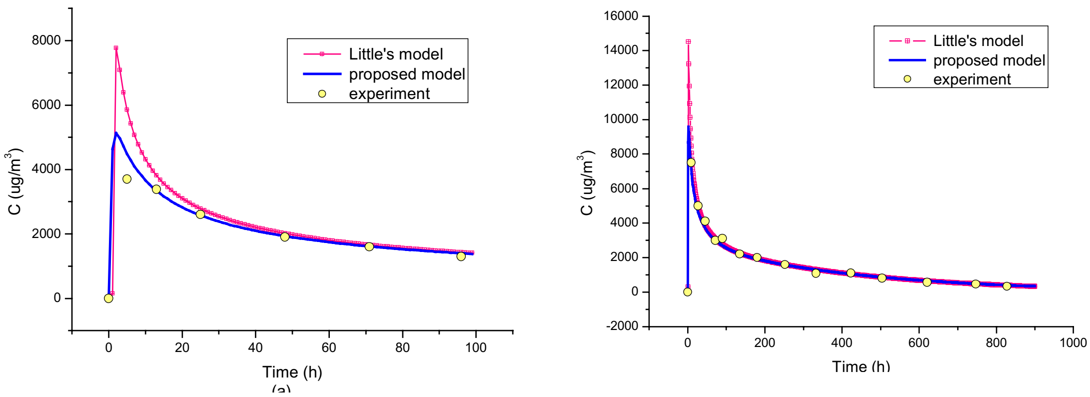
VALIDATION OF THE MODEL

In order to verify the aforementioned model, the predicting instantaneous VOC concentration of a small environmental chamber based upon the model is compared with the experimental results (Yang, 2001). Assuming that the air in the chamber is well-mixed, the VOC mass in chamber air obeys the mass conservation law as follows:

$$\frac{dC_\infty(t)}{dt}\cdot V = A\cdot \dot{m}(t) - Q\cdot C_\infty(t) \tag{10}$$

where A is area of the slab emitting VOC, Q is volumetric air flow rate through chamber.

Combining equations (9) and (10), the instantaneous VOC concentrations of the chamber air can be obtained. The predictions of the proposed model were compared with those of Little's model and experimental data, Fig. 3. It shows that the calculated results by the proposed model agree well with the experimental results. Notice that the model parameters used in the model, were obtained by Yang et al. (1999) through detailed numerical study so the agreement verifies the correct derivation of the new model. On the other hand, Little's model tends to overestimate the chamber air VOC concentration at the early stage of emission as compared with the proposed model and emission test data.



(a) TVOC, PB1 (b) TVOC, PB2

Fig.3 Comparison of the model results and the experimental results for instantaneous contaminant concentration

DISCUSSION

By using the proposed analytical model, the influence of the distribution of initial concentration in building materials on emission characteristics was analyzed through parametric studies. This analysis was done by varying the distribution of initial concentration (uniform, sin curve, cos curve, right triangle and left triangle) in building materials under the condition that the initial VOC mass is equal.The instantaneous emission rate, VOC concentration in chamber air and etc. for the case of the aforementioned TVOC in PB1 tests (Yang et al., 2001), were calculated by using eqs. (6)-(9). The results are schematically shown in Figs.9.

From Figs.9, it is seen that: (1) in the early stage (t<100hours), the effect of initial concentration distribution C0(x) on emission rate is obvious so that the emission mass and chamber compound concentration are strongly influenced by the initial concentration distribution $C_0(x)$; (2) after the period (t ≥ 100 hours), the influences of $C_0(x)$ on emission rate $\dot{m}(t)$, emission mass m(t) and VOC concentration in chamber air decrease with increasing time and they can be neglected in practical application. The reason for those is that at the early stage the VOC concentration in the material surface and the air layer adjacent to the air-material interface are strongly influenced by $C_0(x=0)$ while C(x=0, t) will approach a relatively stable value when time is long enough. For given convective mass transfer coefficient h_m and given slab thickness, the stable value is determined by the ratio of convective mass transfer coefficient to internal mass diffusion resistance and initial VOC content, i.e., the average value of $C_0(x)$. For most building materials with same initial VOC content, if the time is long enough (>100 hours), the internal diffusion mass transfer resistance dominants so that the ratio approaches zero despite whatever the distribution of $C_0(x)$ is. Therefore, the initial VOC concentration distribution only influence the emission characteristics in a short period (<100 hours). Considering the period of VOC emission is much longer than 100 hours, it is justified to neglect the effect of initial VOC concentration distribution on emission characteristics. In other words, for building material with constant thermal physical properties, the long-term (>100 hours) emission characteristics are determined by the initial VOC concentration not by its distribution.

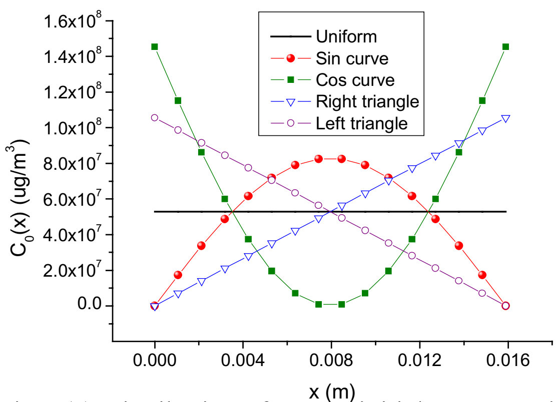


Fig.9 (a) Distribution of TVOC initial concentration

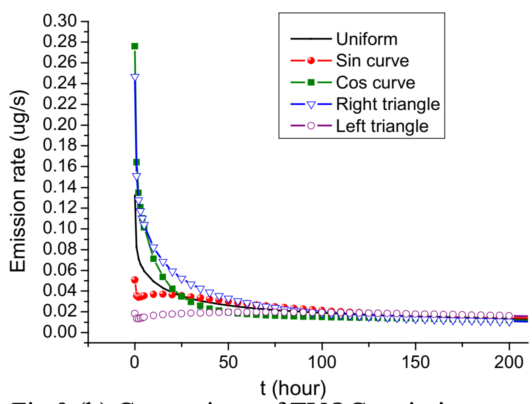


Fig.9 (b) Comparison of TVOC emission rate

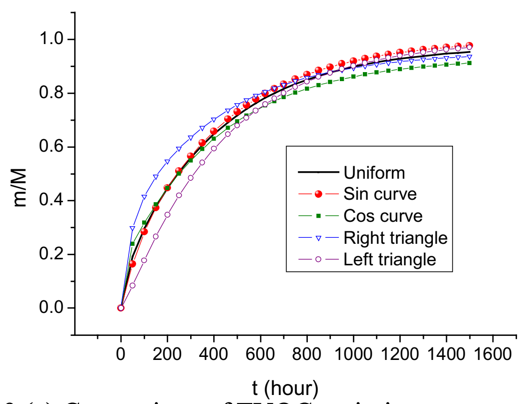


Fig.9 (c) Comparison of TVOC emission mass

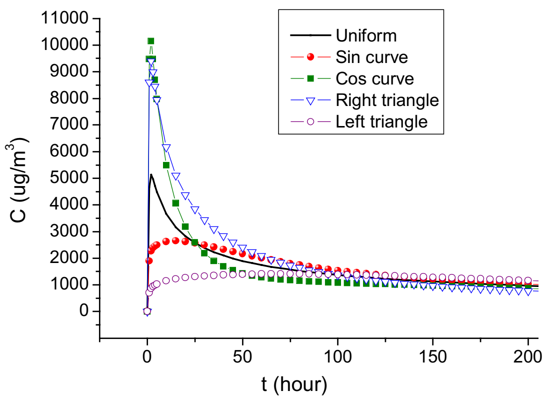


Fig.9 (d) Comparison of TVOC concentration in the chamber air

CONCLUSIONS

Different from the models in the literature, this proposed model considers both the convective mass transfer resistance through the air phase boundary layer and the distribution of initial concentration in building materials. It can precisely predict the emissions of VOCs of indoor material for whole process.The model was validated with experiment. By comparing the results of the proposed model with the results derived from the other model in the literature, it is found that at the early stage, the proposed model agree the experimental data better while after the period, their results are almost the same.

The analysis based upon the proposed model shows that the influence of initial distribution on emission characteristics decreases with increasing time. At the early stage (tends to be shorter than 100 h), the influence is strong and should be considered. After that period, such influence can be neglected. Considering the period of VOC emission of building material used in practical is much longer than 100 hours, it is justified to neglect the effect of initial VOC concentration distribution on emission characteristics.

The proposed model together with the analysis is very helpful to study the VOC emission characteristics and to improve the measurement precision for VOC emission of building materials.

ACKNOWLEDGEMENTS

This work was supported by National Nature Science Foundation of China (The project No. is 50276033) and by Tsinghua University (The project No. is 200007005).

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