

A Unified Conjugate Mass Transfer Model of VOC Emission

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Abstract—This paper develops a unified conjugate mass transfer model for VOC (Volatile Organic Compound) emission, which implies conjugate boundary condition for mass transfer at the material-air interface. Thus, no special treatment is needed at the material-air interface and numerical methods for conjugate heat transfer problem can be applied directly. The material-air partition coefficient has been taken into account and its effect is the same as specific heat in the energy equation. The equivalent diffusion coefficient in the material $K_{ma}D_m$ instead of D_m characterizes the rate of mass transfer. The ratio $K_{ma}D_m/D_a$ indicates whether VOC emission is controlled by the internal diffusion or not. The equivalent air-phase initial concentration C_0/K_{ma} determines the order of maximum concentration in the air. VOC emission contains two stages: the initial stage and the pseudo-steady stage when the emission rate nearly equals mass rate through the outlet of the air. Diffusion coefficient of VOC in the material has a significant effect on VOC emission in the two stages. The effect of partition coefficient on VOC emission depends on the value of $K_{ma}D_m/D_a$.

Key words: Volatile Organic Compounds, CFD, Numerical Model, Conjugate Mass Transfer, Pseudo-steady State

INTRODUCTION

Building materials have been regarded as a major emission source of VOCs (Volatile Organic Compound) in indoor environment. In general, the emission from dry materials has a significant effect on indoor air quality because of their large surface area and permanent exposure to indoor air. Thus, it is important to investigate their influence on indoor air quality so that building materials with low emission rate are used as much as possible.

Up to now, much work has been performed on VOC emission. There exist many measurement results in the literature, which were performed under controlled environmental conditions in environmental test chambers. Since much time and expense is needed for experiments, many researchers turned to mathematical modeling of VOC emission. Little et al. [1994] simulated VOC emission from new carpets using a simplified model and investigated the influence of the material-diffusion coefficient on VOC emission. Sparks et al. [1996] presented an air-phase mass transfer model based on the equivalent air-phase concentration. Huang and Haghighat [2002] used an analytical model and a simplified numerical model to investigate the influence of air velocity on VOC emission. Although these models are based on sound mass transfer mechanism, some prerequisites such as simple boundary and initial conditions cannot be met usually for most cases. Therefore, many researchers turned to CFD (Computational Fluid Dynamics) model to study VOC emission. There are two kinds of techniques to describe the concentration equation. The one technique is to use the gas-phase, liquid-phase and solid-phase concentrations simultaneously in the concentration equation [Choi, 1999; Juncu, 2002]. The other one is to use only the equivalent air-phase concentration as the dependent variable in the concentration equation. Thus, the latter one is consistent with

the conventional solver for partial differential equations. Yang et al. [1998] performed CFD simulation of VOC emission for dry and wet materials. Murakami et al. [1999] used a CFD technique to investigate the emission and sorption of the pollutant emitted from styrene-butadiene rubber floor in the room. Lee et al. [2001] analyzed the behavior of VOCs in an indoor environment by using CFD. Although these models have achieved much success in modeling VOC emission, no partition coefficient is taken into account in these models and the material-air partition coefficient is assumed to be unity. Yang et al. [2001] and Topp et al. [2001] also developed a mass transfer model for VOC emission using two VOC concentrations in the material and the air simultaneously. However, the governing equations were written for multi-domains and conjugate boundary condition for mass transfer at the material-air interface must be given explicitly. Thus, some inconvenience is incurred and a numerical method for conjugate heat transfer cannot be used directly.

In the present study, a unified mass transfer model is developed in which the governing equations are written in a single form for a whole domain with the partition coefficient to be taken into account. By analyzing this model, we can explain the influences of the diffusion coefficient of VOC in the material and the partition coefficient on VOC emission. The present model is applied to a two-dimensional enclosure in the present study.

MATHEMATICAL MODEL

For VOC emission from building materials in rooms, the mass transfer deals with three different regions: the bulk air, the material-air interface and the solid material. At the material-air interface, there exist conjugate boundary conditions, i.e., a continuous mass flux and a concentration jump between the air-phase and material-phase concentration.

The airflow field has much effect on mass transfer because it influences the mass transfer coefficient of air phase [Huang and Hag-

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highat, 2002]. For incompressible flow, the governing equations for flow field can be written as follows:

$$\frac{\partial \rho}{\partial \tau} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (1)$$

$$\frac{\partial}{\partial \tau}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\rho (v + v_i / \sigma_v) \frac{\partial u_j}{\partial x_j} \right] \quad (2)$$

To account for turbulence, the standard k - ϵ turbulence model is adopted.

$$\frac{\partial}{\partial \tau}(\rho k) + \frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j} \left[\rho (v + v_i / \sigma_k) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \epsilon \quad (3)$$

$$\frac{\partial}{\partial \tau}(\rho \epsilon) + \frac{\partial}{\partial x_j}(\rho u_j \epsilon) = \frac{\partial}{\partial x_j} \left[\rho (v + v_i / \sigma_\epsilon) \frac{\partial \epsilon}{\partial x_j} \right] + C_{\epsilon 1} \frac{\epsilon}{k} G_k - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} \quad (4)$$

$$v_i = C_\mu \frac{k}{\epsilon} \quad (5)$$

$$C_\mu = 0.09 \quad C_{\epsilon 1} = 1.44 \quad C_{\epsilon 2} = 1.92 \quad \sigma_k = 1.0 \quad \sigma_\epsilon = 1.3 \quad (6)$$

Eqs. (1)-(6) apply to both the air region and the solid material region. For the solid material region, velocity, kinetic energy and turbulent viscosity will be assigned to be zero.

At the material-air interface, a VOC phase change occurs when it diffuses from the solid material to the room air. Usually, Henry's law is adopted to express the relation between the two concentrations at the material-air interface:

$$C_m|_{i+} = K_{ma} C_a|_{i-} \quad (7)$$

where K_{ma} is the dimensionless material-air partition coefficient and C_m and C_a are the concentrations of VOC in the material and air, respectively. In general, K_{ma} is far from unity, which means that concentration field is discontinuous at the material-air interface. Therefore, the concentration equation applied to air region is different from that applied to solid region. Special care should thus be paid to conjugate boundary condition at the material-air interface. To overcome this difficulty, many researchers [Sparks et al., 1996; Murakami et al., 1999; Lee et al., 2001] introduced the equivalent air-phase concentration to make the concentration field to be continuous.

$$C_{ea} = \begin{cases} C_a & \text{in the air} \\ C_m / K_{ma} & \text{in the material} \end{cases} \quad (8)$$

This means that there exists a corresponding equivalent air-phase concentration for each value of C_m . Substitution Eq. (8) into Eq. (7) yields $C_{ea}|_{i+} = C_{ea}|_{i-}$ at the material-air interface, which means that the equivalent air-phase concentration is continuous in the solution domain. It is helpful to introduce this transformation because the conventional partial differential equation solver is written for a continuous variable. In the present study, the equivalent air-phase concentration will be regarded as the dependent variable in the concentration equation.

According to Fick's law, the mass flux can be described as follows:

$$J = D \frac{\partial C}{\partial x_j} \quad (9)$$

According to the conservation law of mass transfer at the mate-

rial-air interface, there exists

$$J|_{i+} = J|_{i-} \quad (10)$$

Application of Eq. (9) to Eq. (10) yields:

$$\left(-D_m \frac{\partial C_m}{\partial x_j} \right)_{i+} = \left(-D_a \frac{\partial C_a}{\partial x_j} \right)_{i-} \quad (11)$$

where D_m and D_a are the diffusion coefficients of VOC in the material and air, respectively. Using the equivalent air-phase concentration from Eq. (8), Eq. (11) can be rewritten as:

$$\left(-D_m K_{ma} \frac{\partial C_{ea}}{\partial x_j} \right)_{i+} = \left(-D_a \frac{\partial C_{ea}}{\partial x_j} \right)_{i-} \quad (12)$$

Compared with Eq. (11), there is an additional term K_{ma} on the left side of Eq. (12). It yields that Eq. (12) cannot be compatible with the original concentration equation. To eliminate this phenomenon, the equivalent diffusion coefficient is defined as follows:

$$D_{ea} = \begin{cases} D_a & \text{in the air} \\ D_m K_{ma} & \text{in the material} \end{cases} \quad (13)$$

Thus, Eq. (12) can be rewritten as:

$$\left(-D_{ea} \frac{\partial C_{ea}}{\partial x_j} \right)_{i+} = \left(-D_{ea} \frac{\partial C_{ea}}{\partial x_j} \right)_{i-} \quad (14)$$

By this transformation, Eq. (14) is of the same form as Eq. (11). In other words, conjugate boundary conditions, i.e., Eqs. (7) and (11), are converted to Eqs. (8) and (14). The governing equation for concentration can be written as follows:

$$\frac{\partial}{\partial \tau}(K C_{ea}) + \frac{\partial}{\partial x_j}(K u_j C_{ea}) = \frac{\partial}{\partial x_j} \left\{ \left(D_{ea} + \frac{v_i}{\sigma_c} \right) \frac{\partial C_{ea}}{\partial x_j} \right\} + S_c \quad (15)$$

where $K=1$ and $K=K_{ma}$ for air region and solid region, respectively, and σ_c is turbulent Prandtl number for mass transfer and its value is assigned to be 1.0. Obviously, conjugate boundary conditions, i.e., Eqs. (7) and (11), are implied in Eq. (15). If concentration unit is kg/kg, Eq. (15) can be rewritten as

$$\frac{\partial}{\partial \tau}(K \rho_a C_{ea}) + \frac{\partial}{\partial x_j}(K \rho_a u_j C_{ea}) = \frac{\partial}{\partial x_j} \left\{ \rho_a \left(D_{ea} + \frac{v_i}{\sigma_c} \right) \frac{\partial C_{ea}}{\partial x_j} \right\} + S_c \quad (16)$$

Since only one equation is used to describe mass transfer in the present model and no conjugate boundary condition is needed, it would consume less computational time and be easy to understand.

As we know, the energy equation can be written as:

$$\frac{\partial}{\partial \tau}(\rho c_p T) + \frac{\partial}{\partial x_j}(\rho c_p u_j T) = \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) + S_c \quad (17)$$

All parameters such as density, specific heat and thermal conductivity have an effect on heat transfer. Thus, the thermal diffusivity $a = \lambda / \rho c_p$ is related with the rate of temperature change. Obviously the concentration equation has the same form as the energy equation. Thus, numerical methods for a conjugate heat transfer problem can be applied directly to a conjugate mass transfer one. Comparing the concentration equation with energy equation for incompressible flows, we can find that

(1) K in Eq. (15) or Eq. (16) has the same effect as specific heat c_p in Eq. (17).

(2) The diffusion coefficient of VOC in the material $D_m = D_{ea}/K_{ma}$ influences the rate of concentration change in the material.

(3) The larger partition coefficient K_{ma} is, the slower VOC concentration in the solid material changes.

(4) Partition coefficient has little effect on concentration change for the case of low values of D_m .

On the other hand, just like the thermal conductivity scales the rate of heat conduction, the equivalent diffusion coefficient $D_m K_{ma}$, instead of the diffusion coefficient D_m , scales the rate of mass transfer in the solid material. In other words, $D_m K_{ma}$ should be used to scale the ability of VOC diffusion in different materials. Generally, there exist two main mechanisms in VOC emission: the internal diffusion in the material and the surface evaporation to the airflow. For wet materials the latter usually dominates. However, there is not a consistent conclusion for dry materials. In fact, it can be concluded from Eq. (15) or Eq. (16). If the equivalent diffusion coefficient $D_m K_{ma}$ is much smaller than the diffusion coefficient in the air, the emission is controlled by the internal diffusion. If the equivalent diffusion coefficient $D_m K_{ma}$ is of the same order as the diffusion coefficient in the air, the emission is governed by the two factors. And if the equivalent diffusion coefficient $D_m K_{ma}$ is much larger than the diffusion coefficient in the air, the emission is controlled by the surface evaporation.

PROBLEM CONSIDERED AND NUMERICAL PROCEDURE

The studied situation is shown in Fig. 1. The room size is $4.5 \text{ m} \times 3 \text{ m}$. The width of inlet and outlet is 0.02 m . There exists styrene-butadiene rubber (SBR) of 0.005 m thickness on the bottom floor. The VOC emits from SBR and diffuses into the air in a two-dimensional room. The fresh air flows into the room through the inlet and goes out through the outlet. At the inlet, air velocity and VOC concentration are specified. At the outlet, pressure and zero gradients in the normal direction for other scalar variables are specified. No-

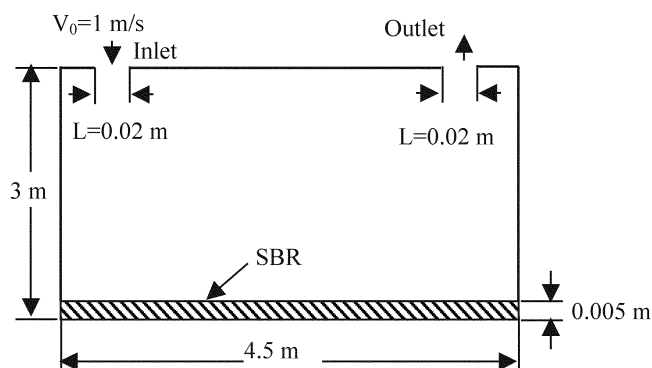


Fig. 1. Room model.

Table 1. Boundary conditions

Inlet	$V_0 = 1 \text{ m-s}$, $k_{in} = 0.02V_0^2$ $\varepsilon_{in} = C_\mu^{0.75} k_{in}^{1.5} / (0.1L)$, $C_{ea, in} = 0$
Outlet	$p = p_{out}$, $\partial C_{ea} / \partial n = \partial \varepsilon / \partial n = \partial k / \partial n = 0$
Wall	$u = v = 0$, $\partial C_{ea} / \partial n = 0$, Wall function

slip condition is used at all walls and zero gradient normal to the wall is specified for VOC concentration. Wall function [Launder and Spalding, 1974] is used to deal with turbulent kinetic energy and its dissipation rate. Specifics are shown in Table 1.

VOC emission is an unsteady problem in nature. In the present study, the initial concentrations in the air and in the solid material are assigned to be zero and $C_0 = 0.192 \text{ kg/m}^3$, respectively. According to Eq. (8), $C_{ea0} = C_0/K_{ma}$ exists in the solid material. In the present study, only new carpets are considered. The diffusion coefficient D_m , the partition coefficient K_{ma} and the initial concentration C_0 can only be obtained from experiment. And some literature offers these data. The diffusion coefficient of VOC in the air is $5.88 \times 10^{-6} \text{ m}^2/\text{s}$.

In the present study, the commercial software FLUENT 6 is used to solve the governing equations. Second-order upwind scheme is used to discretize the convective terms and central difference for diffusion terms. The SIMPLEC algorithm is used for velocity-pressure coupling.

RESULTS AND DISCUSSIONS

In this section, we present the influence of partition coefficient K_{ma} and material-phase diffusion coefficient D_m in the material on

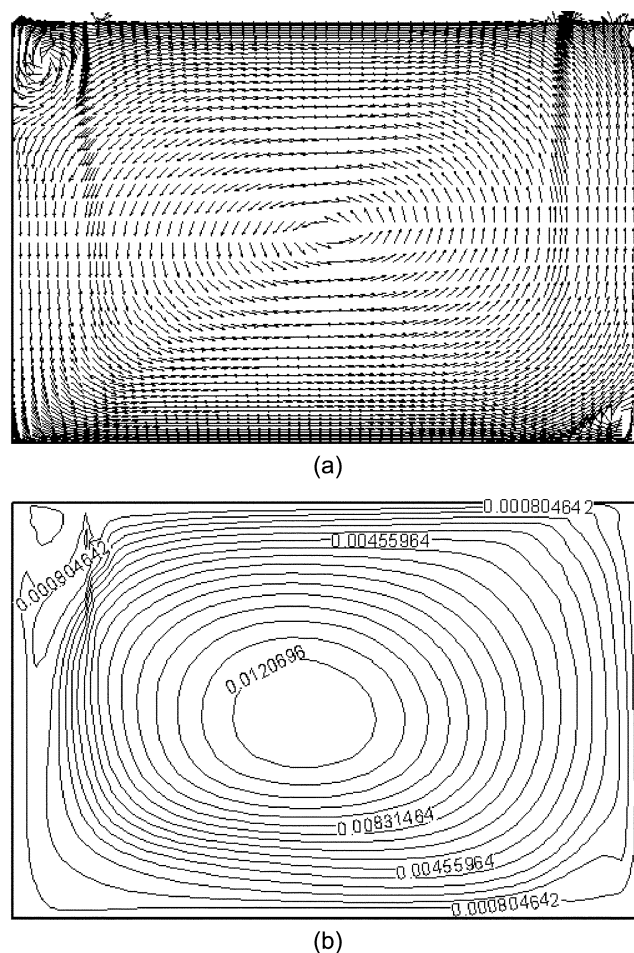


Fig. 2. (a) Velocity vectors in the room. (b) The distribution of turbulent viscosity in the room.

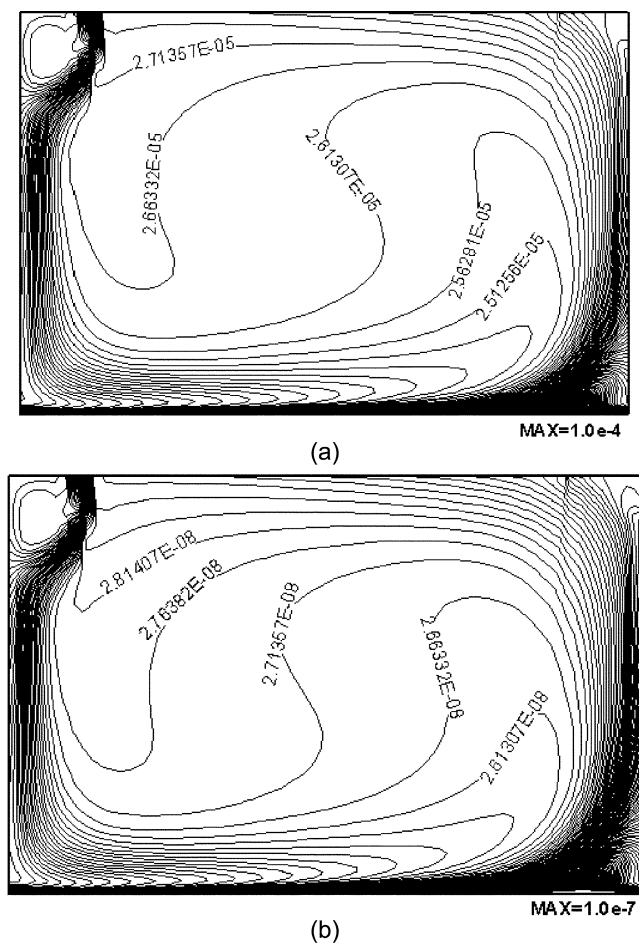


Fig. 3. Concentration contours in the air ($t=48$ h).

(a) $D_m=1.0\text{e-}10$ m²/s, $K_{ma}=1$, (b) $D_m=1.0\text{e-}14$ m²/s, $K_{ma}=1$

VOC emission from dry materials. The influence of age of the material is not taken into account in the present study. Fig. 2 shows the flow field and the distribution of turbulent viscosity in the room. A big vortex is found in the center of the room and some small vortices exist in some room corners. This recirculation in the room helps to make the concentration uniform in the room. On the other hand, there exists strong turbulence in the center of the room, which also promotes the mixing of VOC in the room.

Fig. 3 depicts the concentration fields normalized by C_0 within the room for the two values of D_m . Two figures are similar in shape, which means that the concentration contour is mainly influenced by air flow. The highest concentration occurs on the bottom-right corner of the room, which is in accordance with the airflow pattern. However, the diffusion coefficient in the material greatly affects the values of concentration, which can be seen from the maximum value in the two figures.

The conjugate mass transfer problem is an unsteady one in nature. Fig. 4 depicts the mass flow rate through the outlet and the emission rate from the material and their ratio with time. VOC emission contains two stages: the initial stage and the pseudo-steady stage. In the beginning, the equivalent air-phase concentrations in the air and in the material are zero and C_0/K_{ma} , respectively. Therefore, VOC swiftly transfers from the material into the air and the concentration in the air rises up greatly. With the decreasing of concentration

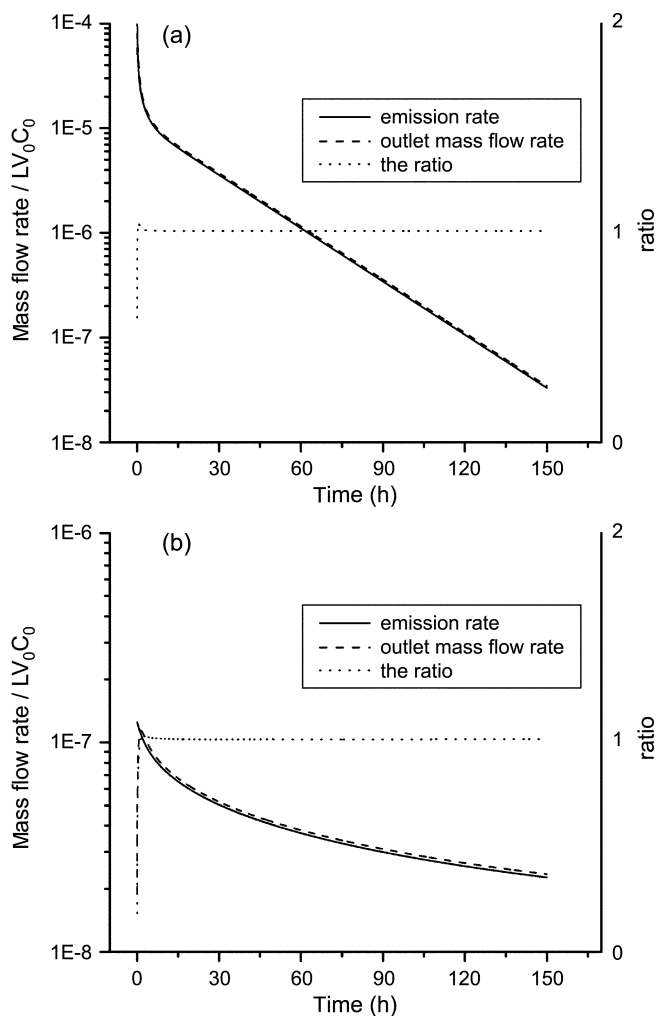


Fig. 4. Outlet mass rate, emission rate and their ratio with time.

(a) $D_m=1.0\text{e-}10$ m²/s, $K_{ma}=1$, (b) $D_m=1.0\text{e-}14$ m²/s, $K_{ma}=1$

difference between the material and air, the mass flow rate through the outlet increases and the emission rate decreases. As shown by Fig. 4, the ratio of the mass flow rate through the outlet to the emission rate at the interface rises up steeply for the two diffusion coefficients. Thus, there would exist a critical time when the emission rate nearly equals the mass flow rate through the outlet. From this time, the net mass flow rate through the boundary of air region remains nearly zero. This stage corresponds to the curve of the ratio nearly to be unity in Fig. 4. Therefore, the concentration field in the air changes very slowly and the average concentration remains nearly the same. In this way, the concentration field in the air arrives at the pseudo-steady stage. Yu and Crump [1998] have pointed out this phenomenon in their review on the emission of VOCs from polymeric materials used in buildings. They called it a 'steady' continuous level and pointed out that the time period for the emission rate to arrive at this stage could vary with the materials. As shown by Fig. 4, this state should depend on the airflow rate also, for the mass flow rate through the outlet is influenced by it.

1. The Influence of the Diffusion Coefficient in the Material

With the same initial concentration Fig. 5 illustrates the effect of D_m on the average concentration in the air with time for different

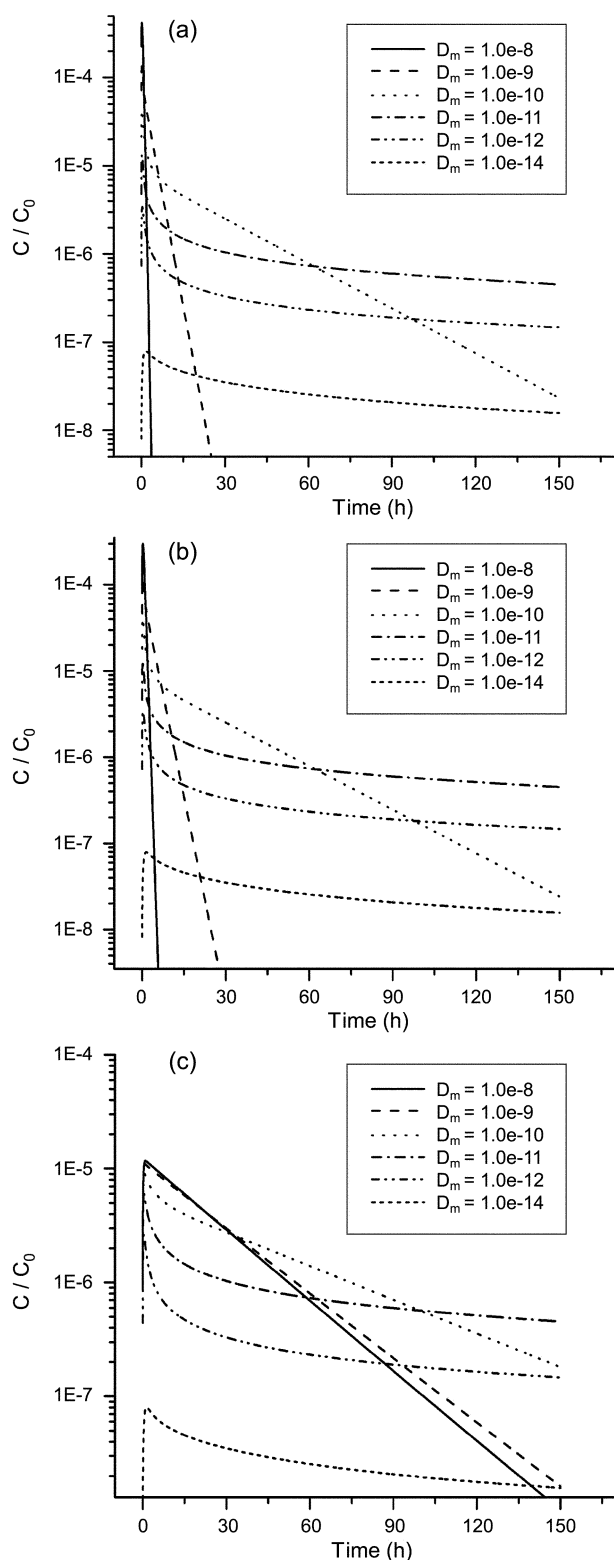


Fig. 5. The influence of diffusion coefficient on the average VOC concentration in the air with time.

(a) $K_{ma}=1$, (b) $K_{ma}=100$, (c) $K_{ma}=10000$

partition coefficients in semi log-log form. All curves depict the same tendency in these curves. Before VOC concentration in the air gets to the peak, a steep line exists and its slope increases with diffusion

coefficient D_m . After the average concentration arrives at the peak, it begins to decrease slowly. After some time, the concentration nearly decreases along a straight line in log-scale. The decreasing rate increases with diffusion coefficients D_m also, which means that the curves for different diffusion coefficients must intersect with each

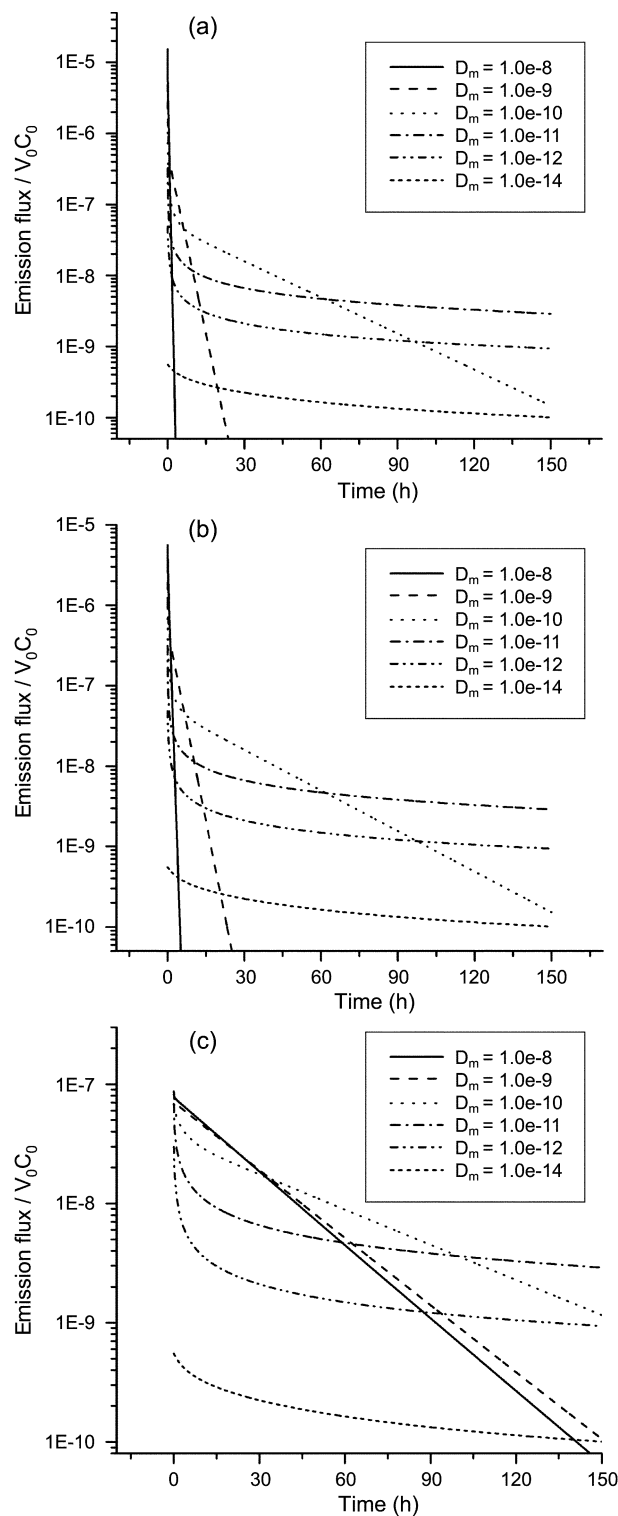


Fig. 6. The influence of diffusion coefficient on the average VOC emission rate with time.

(a) $K_{ma}=1$, (b) $K_{ma}=100$, (c) $K_{ma}=10000$

other after some time. In fact, intersections stand for the conservation of mass transfer because the same initial concentration in the material is used and the integration of all curves should be a constant. As shown by Fig. 5, the curve for $D_m=1.0\text{e-}10\text{ m}^2/\text{s}$ intersects with those for $D_m=1.0\text{e-}11\text{ m}^2/\text{s}$ and $D_m=1.0\text{e-}12\text{ m}^2/\text{s}$ at 60 h and 100 h for the case of $K_{ma}=1$, respectively. We can further conclude that the curve for $D_m=1.0\text{e-}11\text{ m}^2/\text{s}$ will intersect with that for $D_m=1.0\text{e-}12\text{ m}^2/\text{s}$ after a very long time. Curves for $D_m=1.0\text{e-}8$ and $D_m=1.0\text{e-}9$ are also shown in Fig. 5 for comparison, which decrease more rapidly than that of $D_m=1.0\text{e-}10$. Yang et al. [1998] also observed intersections among different diffusion coefficients for a long-term prediction. However, the intersection time in the present study is much smaller than that of Yang et al. [1998], which means that the intersection time may be influenced by airflow and turbulence.

Fig. 6 depicts the effect of D_m on the area-averaged emission flux at the interface with time in semi log-log form. All curves decrease with a very steep line at first. After some time, the decreasing rate begins to reduce. At last a straight line similar to the concentration curve in Fig. 5 exists in Fig. 6 in log-scale. Intersections are also observed in Fig. 6, which is consistent with the concentration curve. Results show that D_m can significantly influence the average concentration and emission rate all along in spite of values of partition coefficient as also obtained by Little et al. [1994] and Yang et al. [1998, 2001]. This may be attributed to that the mass flux is proportional to the diffusion coefficient.

2. The Influence of Partition Coefficient

The influence of partition coefficient K_{ma} on the average concentration in the air is complicated. Since D_m plays a more important role in the governing equation, the effect of K_{ma} on VOC emission is dependent on D_m . Fig. 7 depicts the effect of K_{ma} on the average VOC concentration in the air for different diffusion coefficients in semi log-log form. For the case a), the ratio of D_a to D_m is $5.34\text{e}+4$. In the range of $K_{ma}=1\text{--}1000$, $K_{ma} \ll D_a/D_m$ exists. Here K_{ma} significantly influences the average concentration in the initial stage and does not have much effect on that in pseudo-steady stage, which means that the emission is mainly controlled by the internal diffusion. For $K_{ma}=10000$ where $K_{ma} \ll D_a/D_m$ does not hold, the average concentration is quite different from that of $K_{ma}=1\text{--}1000$, which means that the emission is controlled by both the internal diffusion and surface evaporation. For the case b) where the ratio of D_a to D_m is $5.34\text{e}+6$, the same tendency as case a) is observed. Compared with case a), the difference between the curve of $K_{ma}=1$ and the curve of $K_{ma}=1000$ has been reduced. For the case c) where the ratio of D_a to D_m is $5.34\text{e}+8$, $K_{ma}D_m/D_a$ is so small in the range of $K_{ma}=1\text{--}10000$ that K_{ma} has little effect on the average concentration in the initial stage and pseudo-steady stage. Little et al. [1994] and Yang et al. [2001] also pointed out this phenomenon with diffusion coefficients $D_m=1.0\text{e-}12$ and $D_m=7.65\text{e-}11\text{ m}^2/\text{s}$, respectively. However, the relation between these parameters was not involved.

Fig. 8 illustrates the effect of K_{ma} on the area-averaged emission flux at the interface for different values of D_m . The curves show the same tendency as those in Fig. 7. This means that K_{ma} has little impact on VOC emission for low values of diffusion coefficient D_m , which is in accordance with the model by Sparks et al. [1996]. They presented a simple analytical model to solve the emission flux

$$R=(C_m/K_{ma}-C_a)/(\delta_a/D_a+\delta_m/K_{ma}D_m) \quad (18)$$

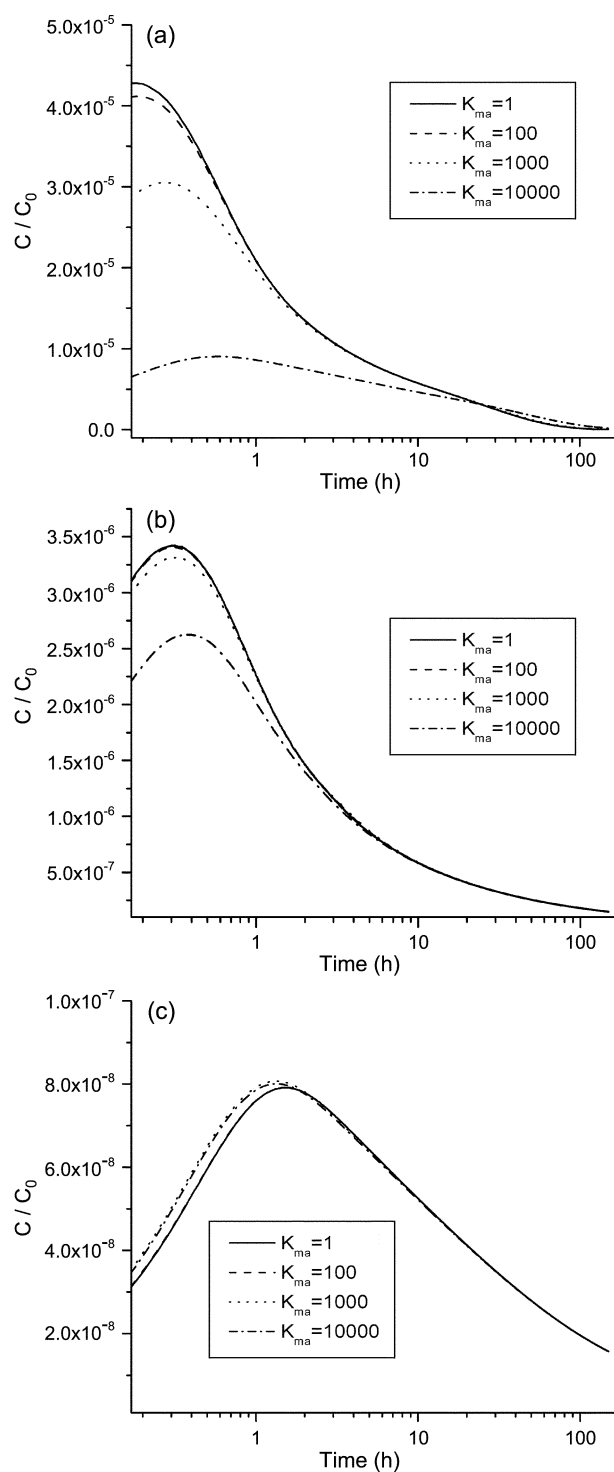


Fig. 7. The effect of partition coefficient on the average VOC concentration in the air with time.

(a) $D_m=1.0\text{e-}10\text{ m}^2/\text{s}$, (b) $D_m=1.0\text{e-}12\text{ m}^2/\text{s}$, (c) $D_m=1.0\text{e-}14\text{ m}^2/\text{s}$

When D_m is so small that $\delta_m/K_{ma}D_m \gg \delta_a/D_a$ exists, the value of R in Eq. (18) can be determined only by D_m and the initial concentration in the material C_0 instead of being influenced by K_{ma} as long as C_a is far smaller than C_m/K_{ma} . In the present study, the above requirements are satisfied by the case of $D_m=1.0\text{e-}14\text{ m}^2/\text{s}$. Table 2 depicts the normalized emission fluxes at the material-air interface

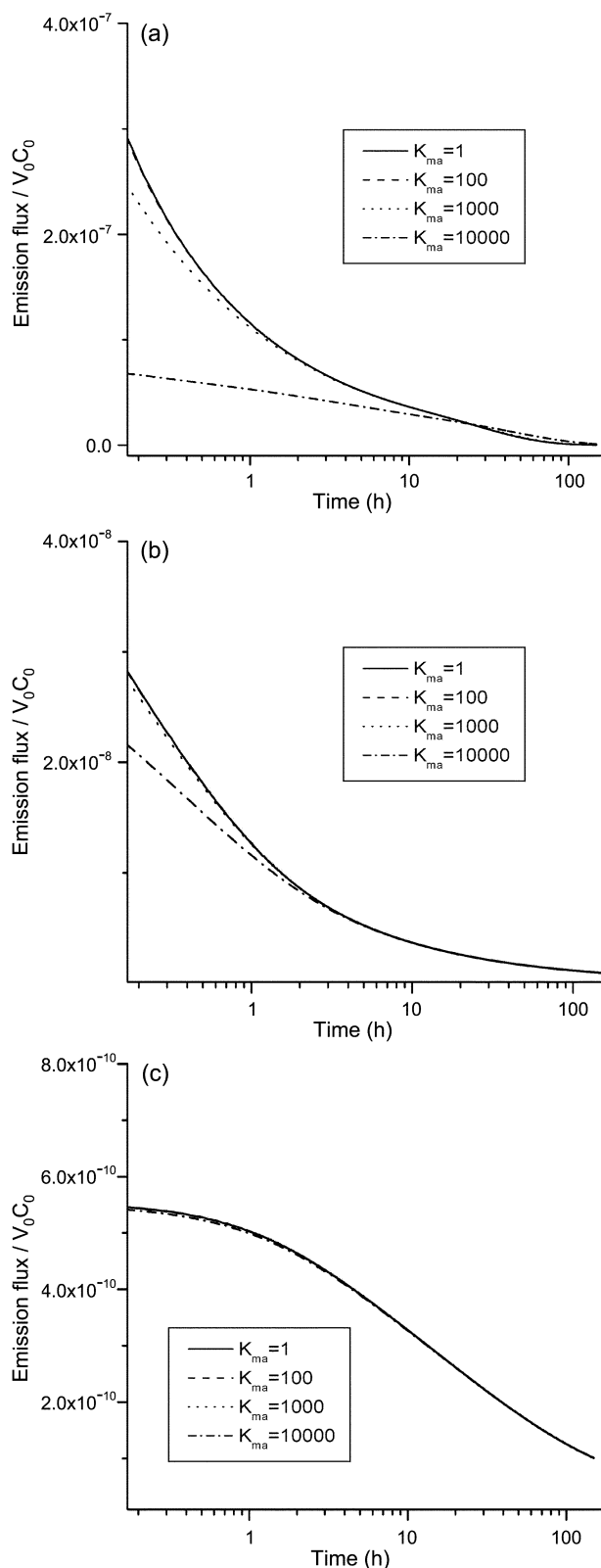


Fig. 8. The effect of partition coefficient on the average emission rate in the air with time.

(a) $D_m = 1.0 \times 10^{-10} \text{ m}^2/\text{s}$, (b) $D_m = 1.0 \times 10^{-12} \text{ m}^2/\text{s}$, (c) $D_m = 1.0 \times 10^{-14} \text{ m}^2/\text{s}$

obtained from the present calculation and from Eq. (18) and relatively good agreement is shown. For the same diffusion coefficient

Table 2. Emission flux at the interface for $D_m = 1.0 \times 10^{-14} \text{ m}^2/\text{s}$

	16 h	32 h	48 h
The present values	2.78e-10	2.14e-10	1.79e-10
The values of Eq. (18)	1.6e-10	1.375e-10	1.28e-10

and initial concentration C_0 , the peak of the average concentration in the air changes with the partition coefficient. According to Eq. (8), the initial equivalent air-phase concentration should be C_0/K_{ma} . According to the second law of thermodynamics, the average concentration in the air should not be more than C_0/K_{ma} . Thus, for a low partition coefficient, there exists a high peak and vice versa. Therefore, C_0/K_{ma} should be used to scale the initial concentration for different materials.

CONCLUSION

This paper presents a unified conjugate mass transfer model based on the equivalent air-phase concentration, which is introduced in Eq. (8) for the entire material region. A conjugate boundary condition at the material-air interface is implied in the governing equation instead of the one written explicitly in Eq. (13), which will consume less computational time. Moreover, in this model numerical methods for a conjugate heat transfer problem can be applied directly to a conjugate mass transfer problem. This model takes a partition coefficient into account completely and the partition coefficient has the same effect as the specific heat in energy equation.

The present study has shown that the equivalent diffusion coefficient in the material, $K_{ma}D_m$, influences the rate of mass transfer and denotes whether VOC emission is controlled by the internal diffusion or not, and that the equivalent air-phase initial concentration C_0/K_{ma} has a strong effect on the maximum concentration in the air. Thus, to scale the VOC diffusion rate and initial concentration in the material, $K_{ma}D_m$ and C_0/K_{ma} should be used. The effect of diffusion coefficient of VOC in the material and partition coefficient on VOC emission has been studied here. The former has a significant effect on VOC emission all along. The effect of the latter on VOC emission depends on the value of $K_{ma}D_m/D_a$. For a low value of diffusion coefficient in the material, the partition coefficient has little effect on VOC emission. However, for a high value of diffusion coefficient in the material, the partition coefficient affects VOC emission only for the short-term emission and has little impact on the long-term one in some range of partition coefficient.

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NOMENCLATURE

- C : concentration [kg/m^3]
- $C_\mu, C_{\epsilon 1}, C_{\epsilon 2}$: turbulence model constants for velocity field
- c_p : specific heat at constant pressure [$\text{J}/(\text{kg} \cdot \text{K})$]
- D : diffusion coefficient [m^2/s]
- G_k : turbulent production term
- J : mass flux [$\text{kg}/(\text{m}^2 \cdot \text{s})$]

K	: equivalent partition coefficient
K_{ma}	: material-air partition coefficient
k	: turbulent kinetic energy [m^2/s^2]
p	: mean pressure [Pa]
S_c	: source term
T	: mean temperature [K]
u	: mean velocity [m/s]
V_0	: inlet velocity [m/s]
x_i	: coordinates [m]

Greek Letters

α	: gas-phase mass transfer coefficient [m/s]
δ_a, δ_m	: distances from the interface to the nearest grid point in the direction of air and solid material [m]
ε	: dissipation rate of k
λ	: thermal conductivity [$\text{W}/(\text{m} \times \text{K})$]
ν, ν_t	: molecular and turbulent viscosities, respectively [m^2/s]
ρ	: density [kg/m^3]
$\sigma_k, \sigma_\varepsilon$: turbulence model constants for diffusion of k, ε
σ_c	: turbulent Prandtl number for mass transfer
τ	: time [s]

Subscripts

a	: air-phase
ea	: equivalent air-phase
i+	: material side of the material-air interface
i-	: air side of the material-air interface
m	: material-phase

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