Coupling finite volume and lattice Boltzmann methods for pore scale investigation on volatile organic compounds emission process

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A coupled numerical model is employed to investigate the emission process of volatile organic compounds (VOCs) in the building material and chamber. In this model, for the first time the Langmuir-isotherm sink model is introduced by taking into account of the adsorption/desorption process between the absorbed VOCs on the material surfaces and the gas phase VOCs in pores. The porous material adopted in the model is reconstructed with a random generation-growth algorithm for 3D microstructures fibers. This model is numerically implemented by a multiscale strategy with the lattice Boltzmann method (LBM) being used to simulate pore-scale diffusion and finite volume method (FVM) for macroscopic transport. Information transferring from the macro scalar obtained from FVM zone to the distribution functions in LBM zone is executed with a reconstruction operator. The model is validated with the well-mixed diffusion model, and then applied to predict the VOCs emission process. A comprehensively investigation of the effects of sorption parameters, including adsorption/desorption rate constants, partition coefficient, Schmidt number and Reynolds number on the VOCs adsorption/desorption process in building material and emission process in chamber is conducted. The simulation results reveal that the equilibrium VOCs concentration in the building material pores could be numerically estimated with our proposed model; the equilibrium concentration of VOCs in a closed chamber depends on the initial emitted VOCs concentration and partition coefficient; Reynolds number can promote the emission process in a ventilated chamber.

1. Introduction

Volatile organic compounds (VOCs) constitute important classes of indoor air contaminants, which are always interacted with almost all the indoor material surfaces. Building material and decorative material have been considered as the main sources of VOCs. Study [1] has shown that the sorption of VOCs and their subsequent desorption contribute substantially to the degradation of indoor air quality (IAQ). Unfortunately, people are unavoidably exposed to building materials in the modern life, and may easily suffer from sick building syndrome [2]. Therefore, predicting the VOCs emissions from building materials is of great importance for risk assessment.

Compared with emission chamber tests, emission simulations by numerical models can provide a more cost effective way to examine the emission behaviors of VOCs. Regarding the whole physicochemical phenomena, the VOCs emission process from the building material to environment is a typical multi-scale process [3], which involves adsorption/desorption process occurring on the microstructure surfaces due to the adsorbability of VOCs, pore-scale diffusion within building material pores at the mesoscopic scale and diffusion/convection in chamber at the macroscopic scale. Most of the existing and commonly used mechanistic models including first order sorption models [1,4,5], single-phase diffusion model [6,7], porous diffusion model [8] and integrated emission and sink model [9,10] are all single scale model, and they have been successfully employed to predict the VOCs emission in the past decades.

Langmuir-isotherm model has been widely adopted as one of the first order sorption models. It assumes that a monolayer of molecules exists on a solid surface and all sorption sites are independent and identical [5]. The sorption rate constants for Langmuir-isotherm model, such as the adsorption/desorption rate constants are obtained by fitting the model constants to
experimental data, which indicates that their accuracy is highly depended on the multiple solutions with different initial estimations [11]. Besides, the model is designed to consider the adsorption/desorption process at the microstructure surface. Therefore, the diffusion process inside the pore space and the chamber cannot be considered in the Langmuir-isotherm model.

The single-phase diffusion model considers the VOCs diffusion in building material and assumes that the VOCs are well-mixed in chamber [6]. Therefore, unlike the Langmuir-isotherm model, the model is computationally intensive but more accurate. In this model, the key parameters, such as effective diffusivity, convective mass transfer coefficient and partition coefficient at the material-phase interface and the initial material-phase compound concentration can highly influence the accuracy of the model [2]. So far, all the parameters are usually obtained with empirical equations or experimental tests and the model does not consider the adsorption/desorption on the material surfaces between absorbed VOCs and gas phase VOCs in the building material.

The porous diffusion model describes the VOCs transport in a porous material, which involves the pores space and solid regions [8]. The adsorption/desorption process is assumed to take place in the whole solid regions, and which is merely handled with the partition coefficient in porous media [2]. This is not proper since the adsorption/desorption process only takes place at the microstructure surfaces. This model is based on the representative elementary volume (REV) scale and seems to be more appropriate in describing the diffusion process in the material since the influence of microstructure on the effective diffusion coefficient is considered [12]. However, as a whole this model is still a macroscopic model in nature, and the results cannot reveal the complex transport process in the material at the pore-scale.

The integrated emission and sink model is a combination of diffusion and sorption model [9,10]. Like the porous diffusion model, this model is also based on REV scale and handles the adsorption/desorption of VOCs as sink/source in the diffusion model.

The information obtained from all the above-mentioned models for VOCs emission transport can predict, in a certain degree, the VOCs emission process correctly. However, in the aforementioned models following two basic questions are not resolved properly and may affect the reliability and applicability of these models.

1. All the models do not consider the influence of real microstructures of the porous material on the VOCs adsorption/desorption process at the pore-scale. The heterogeneous microstructures not only affect the effective diffusion coefficient, but also significantly influence the VOCs adsorption/desorption process. Studies have revealed that VOCs are mainly adsorbed in the micro and meso pore space, and only a small amount of VOCs exists in the macro pore space, which indicate that the microstructure can influence the adsorption/desorption process in building material. According to Xiong et al. [12], for a medium density board (MDB) widely used in China, the pores which occupy the indispensable cumulative pore volume are micro and meso pores, and the pore size diameter is typically below or around 1 μm.

2. All the models above can only partially consider the real VOCs emission process from the building material to the chamber. The first order sorption model ignores the diffusion process in the material pores and chamber, while the single-phase model, porous diffusion model and integrated model ignore or simplify the adsorption/desorption process on the microstructures surfaces.

On the whole, the real emission process is a pore-scale process, which cannot be fully described by the aforementioned models from macroscopic point of view. Besides, some assumptions are usually adopted in these models, such as the VOCs concentration is well-mixed in the room and mass transfer coefficient is usually taken as constant, and does not depend on the air flow rate or the position. Therefore, to understand the VOCs mass transport process in depth, a more fundamental model is highly required which can fully consider the actual structures of building material, the VOCs diffusion in the material pores and the adsorption/desorption process on the material surfaces. The structures of many building material are actually of porous type with pores of different sizes and shapes (see Figs. 1 and 2). The transport process in porous materials can be well simulated by the LBM because of its simplicity and flexibility in dealing with complex boundary conditions [13,14].

Xuan et al. [13] investigated the effective diffusivity of VOCs in a regular and random porous media with LBM. Ma et al. [14] considered the transient desorption process on the material surface, and adopted the Henry law to describe the desorption process between the VOCs and the material. However, the model neglected the adsorption process, thus no equilibrium state can be reached and the VOCs adsorbed on the material and the material pores can be emitted thoroughly, which is not reasonable. However, relatively
2. Simulation methodology

2.1. Mass transport LB model

To quantitatively investigate the effect of microstructures on VOCs emission process in building material, it is necessary to account for the diffusion process at the pore-scale. The LBM is a promising numerical method in computational fluid dynamics for exploring pore-scale phenomena in porous media [13–18]. The LB simulation method employed is based on the Bhatnagar-Gross-Krook (BGK) model, which simulates the mass transport phenomena by tracking the time evolution of concentration distribution functions, and each evolution process contains streaming and collision steps.

The evolution equation of the distribution function is written as

$$f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = \frac{1}{\tau} \left( f_i(x, t) - f_i^{eq}(x, t) \right)$$

(1)

where \( f_i(x,t) \) is the concentration at the site \( x \) and time \( t \), \( \tau \) is the collision time which is related to the mass transfer diffusivity. The equilibrium concentration function is commonly chosen as shown in Eq. (2) [17].

$$f_i^{eq}(x, t) = X \left( \frac{j_i + \frac{1}{2} e_i \cdot u}{j_i} \right)$$

(2)

where \( X \) is the concentration, and \( j_i \) is a specially chosen constant given by Ref. [15]. With the Chapman-Enskog expansion for Eqs. (1) and (2), the advection-diffusion equation can be recovered. We choose a reduced D2Q5 lattice model instead of the original D2Q9 lattice model without loss the accuracy [18].

The discrete velocities are given by

$$e_i = \begin{cases} 0 & i = 0 \\ \left( \cos \left( \frac{(i-1)\pi}{2} \right), \sin \left( \frac{(i-1)\pi}{2} \right) \right) & i = 1, 2, 3, 4 \end{cases}$$

(3)

Species concentration \( X \) is obtained by

$$X = \sum_{i=0}^{4} j_i$$

(4)

\( j_i \) is expressed as

$$j_i = \begin{cases} j_0 & i = 0 \\ \frac{j_0}{(1 - j_0)/4} & i = 1, 2, 3, 4 \end{cases}$$

(5)

with the rest fraction \( j_0 \) can be chosen from 0 to 1.

The diffusivity corresponding to the collision time is written as

$$D = \frac{1}{2} (1 - j_0)(\tau - 0.5) \frac{\Delta x^2}{\Delta t}$$

(6)

where \( D \), \( \Delta x \) and \( \Delta t \) are the diffusivity, lattice step and time increment, respectively.

2.2. Finite volume method

The general governing equation is written as follows:

$$\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma_{\phi} \nabla \phi) + S_{\phi}$$

(7)

where the terms from left side to the right side in Eq. (7) represent the unsteady term, convective term, diffusion term and source term, respectively. \( \phi \) is a scalar dependent variable, \( \Gamma_{\phi} \) is a general
diffusion coefficient. When the variable $\phi$ equals 1, $\mathbf{u}$ and $X$, Eq. (7) represents the continuity equation, momentum equation and mass diffusion equation, respectively. The general governing equation is discretized by FVM. A fully implicit algorithm called IDEAL algorithm is used in this paper to solve the coupling of pressure and the velocity, which overcomes two main assumptions in the SIMPLE algorithm completely [19]. A new stability-guaranteed second-order difference scheme (SGSD) is adopted for the convective term discretion in Eq. (7) [20].

2.3. Concentration coupling distribution functions

In LBM zone, the fluid flow is ignored and only the mass diffusion process is considered in the building materials. In FVM zone, both the mass diffusion and fluid flow are considered in chamber. In the coupled zone, the information derived from the FVM and LBM should be exchanged. It’s worth noting that in the coupled region the solutions of FVM are still of convection-diffusion type. The information calculated from the LBM zone can be easily transformed in chamber. In Fig. 2. It is worth noting that those pore diameters below 1 $\mu$m or over 60 $\mu$m in Ref. [12] are not included due to the grid resolution. As can be seen in this figure, even though some quantitative differences exist, all the PSDs of the reconstructed microstructures show the same distribution trend. The majority of the pore diameters with the reconstruction method is between 15 and 20 $\mu$m, while those in Ref. [12] is around 10 $\mu$m. To the authors’ knowledge such an agreement is acceptable for a stochastic reconstruction method.

Bruggeman equation has been widely adopted to calculate the effective diffusivity $D_{\text{eff}}$

$$D_{\text{eff}} = \frac{\varepsilon}{\tau_{\text{tor}}}$$ (10)

where $\tau_{\text{tor}}$ is the tortuosity, defined as the ratio between the actual flow path length and the straight length of a porous medium. It can be calculated with [22].

$$\tau_{\text{tor}} = (1 + 0.63 \ln(1/\varepsilon))^2$$ (11)

The predicted variations of $D_{\text{eff}}/D$ with the porosity by the analytical model and Ma’s work [14] are also compared with the present study, as shown in Fig. 3. It shows a satisfying accordance among the three methods.

A cross-section of the 3D reconstructed model is chosen and presented in Fig. 4. The length and height of the building material are $L_1 = 1.0 \times 10^{-2}$ m and $H_1 = 1.1 \times 10^{-3}$ m, respectively, and the length and height of the chamber are $L_2 = 1.0 \times 10^{-2}$ m and $H_2 = 1.01 \times 10^{-2}$ m, respectively. The grid resolution in LBM zone is $1.0 \times 10^{-5}$ m, therefore the grid adopted is 1000 x 110; while the grid resolution in FVM zone is 1.0 x 10^-4 m, and the grid adopted is 100 x 101. The chamber is a closed one as $Re = 0$, while it is a ventilated one as $Re \neq 0$. Details of the physical and operation parameters for basic case are listed in Table 1. Note that Schmidt number ($Sc = \nu/D$) defines the ratio of momentum diffusivity and mass diffusivity. The initially absorbed VOCs on the building material surfaces is denoted as $M_{\text{initial}}$. 

In the present study, five microstructures are reconstructed and the porous size distribution (PSD) is statistically determined by the 13 direction averaging method [21]. PSD comparisons of the reconstructed microstructures and the experimental result [12] are illustrated in Fig. 2. The initial VOCs absorbed on the building material surfaces is denoted as $M_{\text{initial}}$. The predicted variations of $D_{\text{eff}}/D$ with the porosity by the analytical model and Ma’s work [14] are also compared with the present study, as shown in Fig. 3. It shows a satisfying accordance among the three methods.

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3.2. Initial conditions and boundary conditions

In order to study the transport process of VOCs from building material to the chamber space, an initial equilibrium state of the VOCs in the building material pores is needed. We proposed a numerical method to predict the initial VOC concentration, which is stimulated from the physical process described in Ref. [23]. The model supposes that at the beginning VOC components exist only in the building material, and then they desorb to the chamber space, an initial equilibrium state of the VOCs concentration is numerically obtained. Then this equilibrium state is taken as the initial condition for the simulation of VOCs emission from building material surface to the chamber space. In the present study, to obtain the initial equilibrium state, only LBM is used for the region of building material; while for the emission process, both LBM and FVM are adopted.

The following lists the detailed initial conditions and boundary conditions of the two computations.

For obtaining the equilibrium state, the initial condition is that the adsorbed VOCs concentration on the material surfaces is \( M_{\text{initial}} \), and the VOCs concentration in the building material pores is 0. The boundary condition is that all the walls of LBM zone are no-flux during this process. The computation ends when an equilibrium state is reached.

For the emission simulation coupled by LBM and FVM, the boundary conditions are as follows.

In FVM zone, no-slip condition and no-flux condition are implemented for all velocities and concentration at the walls. For the inlet as shown in Fig. 4 following conditions are adopted:

\[
X = 0, \quad u = \text{Re}_{\text{ref}}/v, \quad v = 0
\]  

\[
\frac{\partial X}{\partial x} = 0, \quad \frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial x} = 0
\]  

where \( \text{Re}_{\text{ref}} \) is the characteristic length which equals 2 × 10^{-3} m in the present study, and for the outlet,

\[
\text{In the coupled zone, the VOCs concentration at the bottom wall of FVM is calculated with [6,7,24].}
\]

\[
X_{\text{FVM}} = \frac{X_{\text{LBM}}}{K_{\text{part}}}
\]  

where \( K_{\text{part}} \) is the material/air partition coefficient.

The VOCs concentration at the upper wall of LBM used in Eq. (8) is obtained with

\[
X_{\text{LBM}} = \frac{X_{\text{LBM}}}{K_{\text{part}}}
\]  

In LBM zone, bounce back condition of the concentration distribution function is applied on the walls. At the surface of the building material and the pores, Langmuir-Isenthal model is used to describe the variation of VOCs concentration and adsorbed VOCs on the material surfaces. The Langmuir-Isenthal model can be discretized as follows:

\[
\frac{dX(x,t)}{dt} = R( -k_aX(x,t) + k_dM(x,t)),
\]

\[
\frac{dM(x,t)}{dt} = k_aX(x,t) - k_dM(x,t), \quad k_e = \frac{k_d}{k_d} = \frac{M_{eq}(x,t)}{X_{eq}(x,t)}
\]  

where \( X(x,t) \) and \( M(x,t) \) are the VOCs concentration in the pore and the VOCs adsorbed on the material surfaces, respectively. \( R \) is the loading ratio in the MDB and \( k_e \) is the equilibrium constant. The rate constants \( k_a \) and \( k_d \) are obtained from Ref. [1]. Fig. 5 schematically shows the VOCs phases in the building material.

There are two types of VOCs in the domain, namely, absorbed VOCs and gas phase VOCs. Adsorption/desorption process is taken places in the nodes named 1 and 2. For the nodes named 2 there are two adsorption/desorption surfaces while those nodes named 1 is only one adsorption/desorption surface. For brevity, the following equations implicitly present the evolution of the adsorbed VOCs and their nearest VOCs concentration in pores on the basis of Eq. (16):

**Table 1**

Physical parameters and basic case.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>( k_{\text{part}} ) (mm·m⁻³)</th>
<th>( M_{\text{initial}} ) (mg·m⁻²)</th>
<th>( k_a ) (m·s⁻¹)</th>
<th>( k_d ) (s⁻¹)</th>
</tr>
</thead>
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<td>0.25</td>
<td>2.81</td>
</tr>
<tr>
<td>Parameters</td>
<td>( v ) (m·s⁻¹) ( Sc ) ( Re )</td>
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<td></td>
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<td>Value</td>
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<td>50</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
For those nodes named 1

\[ M_1(x, t + \Delta t) = \frac{(1/\Delta t + k_d R)M_1(x, t) + k_a X_{1,1}(x, t)}{1/\Delta t + k_d R + k_d} \]  \quad (17)

\[ X_1(x, t + \Delta t) = X_1(x, t) + R(M_1(x, t) - M_1(x, t + \Delta t)) \]  \quad (18)

For those nodes named 2

\[ X_{2,2}(x, t + \Delta t) = \frac{2X_{2,2}(x, t) + \Delta t \left[ \frac{k_a M_1(x, t)}{1 + k_d} + \left( k_d - \frac{R k}_d + k_d \right) \right] (X_{2,2}(x, t) - X_{2,1}(x, t))}{2 + 2k_d \Delta t R - 2k_d k_d \Delta t^2 R/(1 + k_d \Delta t)} \]  \quad (19)

\[ X_{2,1}(x, t + \Delta t) = X_{2,2}(x, t + \Delta t) + X_2(x, t) - X_{2,2}(x, t) \]  \quad (20)

\[ M_2(x, t + \Delta t) = \left[ M_2(x, t) + \Delta t \left( k_d X_{2,1}(x, t) + k_d X_{2,2}(x, t) \right) \right] / (1 + k_d \Delta t) \]  \quad (21)

3.3. Validation of the model

In order to verify our proposed coupled model, a well-mixed diffusion model developed by Xu et al. [7] is used to estimate the emission process of VOCs in a closed chamber. For brevity, the details of Xu’s model is omitted here. Based upon the basic case listed in Table 1, the model parameters needed in Xu’s model are numerically predicted by our proposed model, and the results are listed in Table 2.

The comparison of the VOCs concentration in chamber is shown in Fig. 6. The result obtained with our proposed model accords well with that of Xu’s model, showing the reliability of the proposed model.

4. Results and discussion

In the following section, the results of the two computations (obtaining the equilibrium state and emission process) are presented together. The effects of adsorption/desorption rate constants, partition coefficient and Schmidt number are firstly investigated, and then the operation parameters are studied. The influence of each parameter is investigated while keeping the other parameters constant, and the values of the parameters of the basic case are listed in Table 1.

4.1. Influence of adsorption rate constant

Fig. 7 presents the VOCs adsorption/desorption process in the building material and emission process in a chamber with different adsorption rate constant \(k_a\). The VOCs concentration increases significantly at the beginning and then tends to be gentle. The equilibrium concentration increases with a decrease in \(k_a\) which is consistent with the results shown in Fig. 7(a). Based on Fig. 7(c), a conclusion can be drawn that the equilibrium VOCs concentration in the material building depends on \(k_a\) and a higher \(k_a\) leads to a lower equilibrium VOCs concentration.

4.2. Influence of desorption rate constant

The influence of desorption rate constant \(k_d\) on the adsorption/desorption process in the building material and emission process in the chamber is investigated and the results are presented in Fig. 8. Fig. 8(a) shows VOCs concentration in material pores during the adsorption/desorption process, the VOCs are all adsorbed on the surfaces of the material and the VOCs concentration in the pores is zero. Therefore, at the beginning desorption process is dominant on the basis of Eq. (16), and the variations of VOCs concentration in pores are nearly the same. When the VOCs concentration is higher, adsorption process becomes more significant. Thus, a higher adsorption rate constant could lead to an equilibrium state earlier. The equilibrium VOCs concentration decreases with a higher \(k_a\) due to a higher equilibrium constant (see Eq. (16)). The adsorbed VOCs on material surfaces during the adsorption/desorption process depicted in Fig. 7(b) shows an opposite variation trend compared with Fig. 7(a). This is mainly because the total amount of VOCs is a constant.

Fig. 7(c) presents the VOCs emission process in a chamber. The VOCs concentration increases significantly at the beginning and then tends to be gentle. The equilibrium concentration increases with a decrease in \(k_a\) which is consistent with the results shown in Fig. 7(a). Based on Fig. 7(c), a conclusion can be drawn that the equilibrium VOCs concentration in the material building depends on \(k_a\) and a higher \(k_a\) leads to a lower equilibrium VOCs concentration.

### Table 2

Model parameters in Xu's model.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>(h_m) (m s(^{-1}))</th>
<th>(c_0) (mg m(^{-3}))</th>
<th>(D_{\text{eff}}) (m(^2) s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
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<td>3.78e-6</td>
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</table>

![Fig. 6. Comparison of the present model and the well-mixed model.](image-url)
adsorption/desorption process. It can be seen clearly that a higher $k_d$ corresponds to a higher VOCs concentration in material pores, and the VOCs concentration increases with $k_d$ exponentially at the initial stage of the adsorption/desorption process. These results can also be easily explained with Eq. (16). Fig. 8(b) depicts the variation of adsorbed VOCs at the material surface with Fourier numbers under different $k_d$. The results indicate that for small values of $k_d$ the absorbed VOCs decreases slightly with $F_o$, while
for large values of \( k_d \) (>28.1 h\(^{-1}\)) the absorbed VOCs decreases significantly at initial stage and then keeps constant with \( F_o \).

Fig. 8(c) presents the VOCs emission process in the chamber under different \( k_d \). The result is similar to Fig. 7(c) that the variation of VOCs concentration increases significantly at the beginning and then tends to be gentle. The equilibrium concentration increases with \( k_d \) due to a lower equilibrium constant \( k_e \). Besides, like the adsorption rate constant, desorption rate constant shows no effect on the time for the chamber to reach an equilibrium state. It is mainly because that the VOCs concentration in the building material has already in an equilibrium state at the beginning of the VOCs emission in chamber, and the amount of VOCs emitted in the chamber is quiet small compared with the total amount of VOCs. Therefore, it is always in a quasi-equilibrium state in building material with different desorption rate constants. Based on Figs. 8(a) and (c), conclusions can also be drawn that the initial emitted VOCs concentration in the material building depends on \( k_d \), and the equilibrium VOCs concentration in chamber depends on the initial emitted VOCs concentration in building material.

4.3. Influence of partition coefficient

Partition coefficient is usually used to describe the concentration relationship at the interface between building materials and chamber (see Eq. (14)). Fig. 9 presents the VOCs emission process in chamber with different partition coefficients. It can be seen that the equilibrium VOCs concentration in chamber is almost inversely varied with the partition coefficient. This is mainly because the VOCs concentration at the interface decreases with partition coefficient. Combining the aforementioned results of partition coefficient and adsorption/desorption rate constants, the following conclusions can be drawn. With the constant absorbed VOCs, the initial emitted VOCs concentration in the building materials depends on the adsorption/desorption rate constants, and the VOCs concentration in the chamber depends on the initial emitted VOCs concentration and partition coefficient.

4.4. Influence of Schmidt number

The influence of Schmidt number on the effect of VOCs adsorption/desorption process in building material and emission process in chamber has been investigated. Fig. 10(a) illustrates the variation of VOCs concentration in material pores with \( F_o \) under different Schmidt numbers. It can be seen that at the initial stage VOCs concentration in the material pores is strongly dependent on Schmidt number, and the higher the Schmidt number the higher the concentration, even though their variation speeds with time are almost the same. However, finally all cases with different Schmidt numbers approach the same equilibrium state. These can be explained as follows. The amount of VOCs desorbed from the microstructure surfaces can be considered as source term \( S_X \) in Eq. (7). The governing equation for mass diffusion in building material can be simplified as:

\[
\frac{\partial (\rho X)}{\partial F_o} = \frac{t^2 \text{ref} \nabla (\nabla X)}{L^2 \text{ref} \text{Sc} S_X} + \frac{\alpha}{\nu}
\]

(22)

As can be seen in Eq. (22), a lower Schmidt number corresponds to a lower source term. Therefore, the variation of VOCs concentration in the building material increases with Schmidt number. The equilibrium VOCs concentration only depends on the adsorption/desorption rate constants, therefore, all cases reach the same equilibrium state in the end.

Fig. 10(b) depicts the VOCs concentration in the chamber during emission process. It can be seen that Schmidt number has no
influence on the variation of concentration in chamber (seen in Eq. (22)), which accords well with the results of [24].

4.5. Influence of Reynolds number

The influence of inlet Reynolds number on the VOCs emission process in chamber is investigated and Fig. 11 presents the results. The equilibrium state can be reached earlier with a higher Reynolds number. Besides, the equilibrium concentration in chamber decreases with an increase in Reynolds dramatically. This is mainly because VOCs flows out of the chamber, and the mass transfer coefficient at the interface between chamber and building materials increases with Re. Fig. 12 shows the VOCs concentration and stream line with different Reynolds numbers. It can also be found that VOCs distributes unevenly in chamber. Combing the influences of Schmidt number and Reynolds number on VOCs concentration in the chamber, it can be concluded that VOCs concentration would be changed greatly with operation conditions (such as inlet Reynolds number) in an open chamber. However, in a closed chamber, equilibrium concentration would not be influenced by Schmidt number, and the parameters influencing the emission source term would influence emission rate (such as Schmidt number).

Fig. 11. VOCs emission process with different Reynolds numbers.

Fig. 12. VOCs concentration and steam line with different Reynolds numbers.
5. Conclusions

In the present study, a new VOCs emission model is proposed, which considers adsorption/desorption on the material surface and the diffusion in the material pores and chamber. A multiscale process approach is adopted in which LBM is used to simulate pore-scale diffusion in the building material and FVM is used to investigate the macroscopic transfer in the chamber. A numerical method is proposed to estimate the initial equilibrium VOCs concentration in building material. The main conclusions are as follows:

1. According to the proposed numerical method the initial equilibrium VOCs concentration in building material increases with desorption rate constant and decreases with adsorption rate constant;
2. VOCs concentration in chamber is inversely varied with the partition coefficient;
3. Variation of material pores increases with Schmidt number, and Schmidt number has no influence on the variation of concentration in chamber;
4. Equilibrium state can also be reached earlier with a higher Reynolds number, and the equilibrium concentration in chamber decreases with the increase in Reynolds dramatically.

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References