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A NEW HYBRID ALGORITHM FOR NUMERICAL SIMULATION OF VOC EMISSIONS USING SINGLE-LAYER AND MULTILAYER APPROACHES

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A new hybrid algorithm based on the lattice Boltzmann method (LBM) and the finite-volume method (FVM) is proposed for numerically calculating the emissions of volatile organic compounds (VOCs) from building materials and predicting their space distribution. Most building envelopes are comprised of single as well as multilayer materials, with some of them being porous and others nonporous. First, only the LBM is used to calculate the VOC concentration in airtight and ventilated chambers with constant as well as variable ventilation. For multilayer materials, including both porous and nonporous, half-lattice division methodology in the LBM is used, which ensures flux continuity at the interfaces. Good agreement is found between computed results and experimental data available in the literature. The effect of variable ventilation is also studied for both types of sequences of porous/nonporous layers. Then the LBM coupled with the FVM is used to investigate the VOC concentration distribution in the room emitted from styrene-butadiene rubber (SBR) plate, and good agreement is found between obtained results and those already published. The hybrid algorithm with multilayer approach is also used to conduct a detailed study of the effect of different ventilation organizations on the concentration in the room air, and the best one is found by the simulation.

1. INTRODUCTION

Indoor air quality is quite a critical issue for public health because a lot of people in the developed countries spend up to 90% of their time in indoor environment, and workers/employees work in offices up to 60% of their time [1]. Many studies have shown that commonly used materials such as wood products, floor coverings, wall coverings, etc., emit a variety of volatile organic compounds.
compounds (VOCs), which seriously reduce the indoor air quality (IAQ). One way to improve IAQ is to organize ventilation appropriately. Different workplaces have different ventilation positions. So, it is important to investigate the VOC emissions from building materials and their distribution with different ventilation organizations. Most building and furniture envelopes are comprised of single as well as multilayer materials which act as sources of VOCs. These building materials may include both wet and dry materials such as carpeting, wallpaper, gypsum board, paint, and glue. Indoor air quality is considerably affected by the emission of VOCs from dry building materials, as not only the emission is a long-time process but their large surface areas are permanently exposed to indoor air [2].

The internal microstructure of dry building materials can be divided into porous and nonporous ones. Most building materials are somewhat porous, e.g., wood, concrete, ceiling tiles, plaster, and gypsum board, while metal, glass, and hard plastics can be taken as nonporous.

Upto now, a lot of work has been done on measurement of VOC emissions. A majority of the tests use a small-scale test chamber under controlled environmental conditions. Such measurements are very important in order to accumulate and compile a reliable database of indoor materials. However, both the geometry and boundary conditions in buildings may be different from the test sample. Hence, the measured data from a chamber may not be fully suitable for real buildings. On the other hand, with the rapid development of computer hardware and numerical algorithms, mathematical models and numerical simulations can partially overcome the disadvantage of laboratory measurements and can be a useful complement and extension. In this regard, Little et al. [3] first developed a simple but effective diffusion-control model for VOC emissions from a carpet. In this model, boundary-layer resistance and sink effect of the chamber wall were neglected. VOC concentration in both the air phase and the material was calculated by the model, for which the diffusion coefficient, partition coefficient, and initial VOC concentration were obtained from experiment data.

**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(b)</td>
<td>initial material thickness, m</td>
</tr>
<tr>
<td>(c)</td>
<td>lattice streaming speed</td>
</tr>
<tr>
<td>(C_a)</td>
<td>VOC concentration in the air, (\mu g/m^3)</td>
</tr>
<tr>
<td>(C_{a, \text{int}})</td>
<td>air-phase/side VOC concentration in the first near-interface grid, (\mu g/m^3)</td>
</tr>
<tr>
<td>(C_{as})</td>
<td>VOC concentration in the air near the material surface, (\mu g/m^3)</td>
</tr>
<tr>
<td>(C_{in})</td>
<td>VOC concentration in the supply air, (\mu g/m^3)</td>
</tr>
<tr>
<td>(C_{m, \text{int}})</td>
<td>VOC surface concentration on the material side, (\mu g/m^3)</td>
</tr>
<tr>
<td>(C_0)</td>
<td>initial VOC concentration in the material, (\mu g/m^3)</td>
</tr>
<tr>
<td>(D_a)</td>
<td>diffusion coefficient in the air, (m^2/s)</td>
</tr>
<tr>
<td>(D_{a, \text{int}})</td>
<td>diffusion coefficient on the air side, (m^2/s)</td>
</tr>
<tr>
<td>(D_m)</td>
<td>diffusion coefficient of the material, (m^2/s)</td>
</tr>
<tr>
<td>(D_{m, \text{int}})</td>
<td>diffusion coefficient on the material side, (m^2/s)</td>
</tr>
<tr>
<td>(f_{eq})</td>
<td>equilibrium distribution function</td>
</tr>
<tr>
<td>(h)</td>
<td>lattice distance</td>
</tr>
<tr>
<td>(h_m)</td>
<td>mass transfer coefficient, m/s</td>
</tr>
<tr>
<td>(K_{ma})</td>
<td>material/air partition coefficient</td>
</tr>
<tr>
<td>(L)</td>
<td>material loading factor, 1/m</td>
</tr>
<tr>
<td>(N(t))</td>
<td>air exchange rate, 1/s</td>
</tr>
<tr>
<td>(q_{a, \text{int}})</td>
<td>mass transfer rate on the air side, (\mu g/m^2 s)</td>
</tr>
<tr>
<td>(q_{a})</td>
<td>mass transfer rate at the interface, (\mu g/m^2 s)</td>
</tr>
<tr>
<td>(q_{m, \text{int}})</td>
<td>mass transfer rate on the material side, (\mu g/m^2 s)</td>
</tr>
<tr>
<td>(t)</td>
<td>time, s</td>
</tr>
<tr>
<td>(\tau)</td>
<td>relaxation time</td>
</tr>
</tbody>
</table>
In terms of modeling of VOC concentration in a room/chamber, broadly speaking, two types of numerical models are used, i.e., single-zone (well-mixed) models, and computational fluid dynamics (CFD) models. In single-zone models the VOCs in the room are assumed to be well mixed, hence the lumped method is used to predict its averaged concentration in the room. Huang and Haghighat [4] reported an improved single-zone model by considering the boundary-layer resistance, which was neglected in the model of Little et al. [3], and it effectively enhanced the accuracy of the prediction of VOC emission in the initial period. In their model the governing equations were solved by finite-difference technique. In order to investigate the source and sink behavior of diffusion-controlled building materials, Kumar and Little [5] presented a single-layer diffusion model. In their model, the sink effect of the chamber wall and uneven material-phase concentration were considered. Although these models are developed on the basis of a sound mass transfer mechanism, in most practical cases the basic conditions, such as simple boundary and initial conditions, usually cannot be achieved. Considering the fact that most building materials are composed of many layers, Little and Kumar [6] for the first time presented a double-layer model. Their model dealt with the source/sink behavior of layered building materials, and they recommended using a thin barrier layer in order to reduce the rate of emissions. Zhang and Niu [7] developed a multicomponent, multilayer model in which they investigated how various construction materials in multilayer walls, and the different convective mass transfer coefficients between room air and various building components, affect the emission characteristics. After that, Li and Niu [8] presented an integrated mass transfer–based model to simulate different building components, such as floor, ceiling, and walls, composed of porous and nonporous materials. The impact of several ventilation schemes on indoor air quality was also investigated. The main drawback of all these multilayer models is the assumption of uniform distribution of VOC in the room/chamber; i.e., they are all single-zone models, which is actually not achievable in real buildings. Therefore, many researchers turned to CFD model to study VOC emission and its concentration distribution in detail.

In the CFD models, two types of techniques are usually employed in order to describe the concentration equation. In the first technique the gas-phase, liquid-phase, and solid-phase concentrations are used simultaneously in the concentration equation. In the second type, only equivalent air-phase concentration is used as the independent variable in the concentration equation. Murakami et al. [9] introduced the equivalent air-phase concentration and effective diffusion coefficient for the solid region to overcome the discontinuity at the material–air interface. The adsorption/desorption on the side walls by emission from source materials by using CFD technique was studied. Yang et al. [10], developed a CFD technique for the simulation of VOC emission from dry and wet materials. Effects of environmental conditions on both short- and long-term emissions from wet and dry materials have been studied in detail. In all these models the material–air partition coefficient is assumed to be unity. Yang et al. [2] also developed a mass transfer model using CFD approach to predict the internal diffusion, surface emission, and concentration in air. The governing equations were solved for a multidomain by using a conjugate boundary condition for mass transfer at the material–air interface. Kim et al. [11] reported a multiphase model for VOC emission from single-layer building materials and studied...
the effect of different parameters, especially the dependence of effective diffusion coefficient on porosity, in different ways.

The emission in airtight (air exchange being zero) chambers has become a current research problem. Wang and Zhang [12] performed a series of experiments to investigate the formaldehyde emissions from several kinds of medium-density boards (MDF) in a small-scale chamber of 30 L under controlled conditions of 26°C and 30% relative humidity. The important feature of this case is that there is no ventilation, i.e., \( N(t) = 0 \). Xiong et al. [13] developed a general analytical model for formaldehyde emission in both ventilated and airtight chambers. Laplace transfer technique was used to obtain the analytical solution for the problem. Keeping the conditions and data the same as employed by both of the above authors, the lattice Boltzmann method (LBM) is used here to predict the VOC concentration in an airtight chamber, and results are compared with their experimental data.

For simulation of diffusion and convection of heat and mass transfer problems, the LBM has become a very popular and successful tool in the past decade [14–18]. To the authors’ knowledge, at the present time there is no publications in the open literature for detailed numerical analysis of VOC emissions using the LBM for an airtight chamber and multilayer building materials. In this article, both the LBM and the finite-volume method (FVM) will be used to predict VOC emissions and effects of ventilation.

For a single-zone model, the LBM is first used for diffusion through single as well as multilayer materials, comprised of porous and nonporous layers. The effect of sinusoidal ventilation is also studied for both types of sequences of porous/nonporous layers. Then the LBM is coupled with the FVM, and is used to investigate the VOC concentration distribution in the room emitted from styrene-butadiene rubber (SBR) plate. Finally, the proposed hybrid method is used to consider the effects of different ventilation positions on the concentration in the room air.

The rest of the article is organized as follows. In Section 2 the mathematical model, both the LBM and the FVM, is briefly introduced. Validation of the present hybrid algorithm is presented in Section 3. Section 4 gives the simulated results, and some conclusions are provided in Section 5.

2. MATHEMATICAL MODEL

The model setup here is used for simulating the diffusion of VOCs from single- as well as multilayer building materials.

The modified Fick’s second law can be used to describe the VOC diffusion in porous and nonporous building materials [19]:

\[
(\varepsilon + K_s) \frac{\partial C_j(y,t)}{\partial t} = D_{s,j} \frac{\partial}{\partial y_j} \left( \frac{\partial C_j(y,t)}{\partial y_j} \right)
\]  

(1)

where \( y \) is distance from bottom to top, \( t \) is time, and subscript \( j \) means the \( j \)th layer, where for the single-layer approach the value of \( j \) is 1. For nonporous materials, \( \varepsilon = 0, K_s = 1 \), \( C \) and \( D_s \) are material-phase concentration and diffusion coefficient, respectively, whereas for porous materials, \( \varepsilon \) is porosity, \( K_s \) is sorption coefficient,
2.1. Lattice Boltzmann Solver

During the last two decades, the lattice Boltzmann method has been adopted as an alternative and powerful numerical scheme for a variety of fluid transport phenomena [20]. Unlike conventional CFD methods, which solve discrete forms of the mass, momentum, and energy conservation equations based on macroscopic quantities such as velocity and density, the LBM uses a more fundamental quantity called the particle velocity distribution function (PDF). This method bridges the gap between the microscopic and the macroscopic worlds. The most important advantages of the LBM are the easy implementation of complex geometry boundary conditions and multiple interparticle interactions, and in general, computational law can hold automatically without additional computational efforts [21, 22]. Over the years the LBM has been developed successfully for simulations of hydrodynamics and thermophysics for porous materials [15, 18, 23–25]. The development of multiphase conjugate boundary conditions is a recent trend and contemporary research has proved that the LBM is much more efficient than the finite-difference method (FDM) even for problems with very simple geometry [17].

In the LBM the dependent variable is the distribution function \( f_k(y, t) \) of species [15, 16, 26], which is governed by following transport equation:

\[
\frac{\partial f_k(y, t)}{\partial t} + c_k \frac{\partial f_k(y, t)}{\partial x} = \Omega_k \quad k = 1, 2, 3, \ldots, M
\]

(2)

where \( f_k \) is the particle distribution function which streams along lattice link \( h = c_k \Delta t \) with velocity \( c_k \) connecting the nearest neighbors, and \( M \) is the total number of directions in a lattice through which information is propagated. The term \( \Omega_k \) represents the rate of change of the distribution function due to collision.

By using the Bhatnagar-Gross-Krook (BGK) approximation, the collision operator can be written as

\[
\Omega_k = -\frac{1}{\tau} [f_k(y, t) - f_{eq}^k(y, t)]
\]

(3)

where \( \tau \) is the relaxation time and \( f_{eq}^k(y, t) \) is the equilibrium distribution function.

For the case of VOC diffusion problems, the equilibrium distribution function is given by

\[
f_{eq}^k(y, t) = w_k C(y, t)
\]

(4)

where \( w_k \) are the weights which satisfy the condition of \( \sum_{k=1}^{M} w_k = 1.0 \).

The VOC concentration at any grid point can be related to the distribution function \( f_k \) as

\[
C(y, t) = \sum_{k=1}^{M} f_k(y, t)
\]

(5)
In this article, for diffusion of VOCs in the material, the D1Q2 lattice model has been used as shown in Figure 1. In the figure, nodes 2, 3, ..., n - 1 are internal nodes, whereas node 1 and n are boundary nodes. The above LB transport equation for the given case can be discretized as

\[ f_k(y + \Delta y, t + \Delta t) - f_k(y, t) = -\frac{\Delta t}{\tau} [f_k(y, t) - f_k^{eq}(y, t)] \quad k = 1, 2 \]  

The lattice velocities and their corresponding weights are as follows:

\begin{align*}
    c_1 &= v \\
    c_2 &= -v \\
    w_1 &= w_2 = \frac{1}{2}
\end{align*}

Also, \( v = h/\Delta t \), where \( h \) is lattice distance. The relaxation time \( \tau \) can be computed as

\[ \tau = \frac{D_{eff} \Delta t}{v^2 + \frac{\Delta t}{2}} \]  

where \( D_{eff} = D_s/(\varepsilon + K_s) \), and \( \Delta t \) is the time step.

The discretized form of the LB transport equation for \( f_1 \) and \( f_2 \) is

\begin{align}
    f_1^{j+1} &= \left( 1 - \frac{\Delta t}{\tau} \right) f_1^j + \frac{\Delta t}{\tau} f_{1j}^{eq,t} \quad j = 1, 2, \ldots, n - 1 \\
    f_2^{j+1} &= \left( 1 - \frac{\Delta t}{\tau} \right) f_2^j + \frac{\Delta t}{\tau} f_{2j}^{eq,t} \quad j = n, n - 1, \ldots, 2
\end{align}

By splitting the solution algorithm for Eq. (9) into two steps:

**Collision step:** The right-hand sides of Eq. (9) for each node are computed as

\begin{align*}
    f_1^{j+1} &= \left( 1 - \frac{\Delta t}{\tau} \right) f_1^j + \frac{\Delta t}{\tau} f_{1j}^{eq,t} \quad j = 1, 2, \ldots, n \\
    f_2^{j+1} &= \left( 1 - \frac{\Delta t}{\tau} \right) f_2^j + \frac{\Delta t}{\tau} f_{2j}^{eq,t} \quad j = 1, 2, \ldots, n
\end{align*}  

![Figure 1. D1Q2 lattice.](image-url)
Streaming step: In this step the obtained values are assigned to corresponding nodes.

\[
\begin{align*}
 f_{ij+1}^{t+\Delta t} &= f_{ij}^{t+\Delta t} \quad j = n - 1, \ldots, 1 \\
 f_{ij-1}^{t+\Delta t} &= f_{ij}^{t+\Delta t} \quad j = 2, 3, \ldots, n
\end{align*}
\] (11)

It is clear that the values of \(f_{11}^{t+\Delta t}\) and \(f_{2n}^{t+\Delta t}\) need to be known, which are obtained from the boundary conditions.

2.2. Condition at Material–Air Interface

At the material–air interface, two types of approaches are generally used. The first one is a conventional convection approach with a third kind of boundary condition:

\[
-D_s \frac{\partial C(y, t)}{\partial y} \bigg|_{y=b} = h_m[C_m(t) - C_a(t)]
\] (12)

where the mass transfer coefficient should be taken from references. This approach is much easier to implement than the other one, but the main problem is to find an accurate mass transfer coefficient \(h_m\). Another drawback of this approach is the assumption of uniform distribution of VOCs in the room, represented by \(C_a(t)\), which is actually not achievable in real buildings. However, this approach is adopted here, in a wide range of VOC problems, to verify the validity of the present LBM.

In the second approach, the conjugated mass transfer boundary condition, also called the fourth-kind boundary condition [27, 28], is adopted at the fluid–solid interface to solve the governing equations for fluid flow and mass transfer:

\[
q_{m, \text{int}} = q_{a, \text{int}}
\] (13)

where \(q_{m, \text{int}}, q_{a, \text{int}}\) are the mass fluxes at the interface determined from the material side and from the air side, respectively, and can be calculated as

\[
q_{m, \text{int}} = D_s \frac{C_m - C_{m, \text{int}}}{\Delta y_m}
\]

\[
q_{a, \text{int}} = D_a \frac{C_{a, \text{int}} - C_a}{0.5 \Delta y_a}
\] (14)

where \(C_{m, \text{int}}, C_{a, \text{int}}\) are the interface concentrations calculated from the air side and the material side, respectively. From the continuity consideration, \(C_{m, \text{int}} = C_{a, \text{int}}\), and in our case the two concentrations are related by the partition coefficient, as will be shown later. This approach requires solving mass transfer and fluid flow in both the solid and fluid; the LBM is used for VOC diffusion through the material and coupled with the FVM, which is employed to calculate the VOC concentration in the air. The weakness of this approach is the discontinuity of density at the material–air interface, as the density of the material is much larger than the density of air. This flaw can be removed by taking interface diffusivity as given in Eq. (17).
The mass transfer rate at the material–air interface can also be written in a conventional form as

\[ q_{m,\text{int}} = q_{a,\text{int}} = D_{\text{int}} \frac{C_m - C_a}{0.5 \Delta y_a + \Delta y_m} \]  

(15)

where \( D_{\text{int}} \) is the interface diffusivity, and \( C_m, \Delta y_m \) and \( C_a, \Delta y_a \) are concentrations of VOCs and distances on the materials and air side, respectively. The nodes arrangement is shown in Figure 2.

The relation between two concentrations at the material–air interface for both porous and nonporous materials cases can be described by the linear isotherm approximation:

\[ C_{m,\text{int}} = K_{ma} C_{a,\text{int}} \]  

(16)

where \( K_{ma} \) is the material–air partition.

By using Eq. (14), Eq. (15), and Eq. (16), the final expression of \( D_{\text{int}} \) is obtained:

\[ D_{\text{int}} = \frac{D_s D_a (\Delta y_m + 0.5 \Delta y_a)}{D_a \Delta y_m + K_{ma} D_s (0.5 \Delta y_a)} \frac{(C_m - K_{ma} C_a)}{(C_m - C_a)} \]  

(17)

For porous materials, \( K_{ma} = 1 \), which indicates that the gas-phase concentration is continuous at the material–air interface. In this way the above relation of \( D_{\text{int}} \) gets simplified and becomes “harmonic diffusivity” similar to the one derived by Patankar [29], while solving problems with variable diffusivity.

It should be noted that the lattice point which lies on the interface needs to be specially treated. Every lattice in the material has the same diffusivity, except the lattice on the interface, which has \( D_{\text{int}} \). The special treatment of the surface lattice point will be presented later in detail.

At the material–air interface, the Neumann type of boundary condition is used:

\[ -D_{\text{int}} \frac{\partial C}{\partial y} = q_{\text{int}} \]  

(18)
Equation (12) and Eq. (18) can be used to get the expression of $f_{i+M}^{t'}$ for both of the above-mentioned approaches (convective mass transfer and conjugated mass transfer).

At the bottom of the material the adiabatic condition, i.e., zero flux condition, is adopted:

\[
\begin{align*}
    f_{1}(1) &= f_{1}(2) \\
    f_{2}(1) &= f_{2}(2)
\end{align*}
\]

(19)

2.3. Condition at Material–Material Interface

The mass transfer at the interface between layers of two different materials is handled by using the half-lattice division approach [17]. The interface is placed not exactly on the surface nodes but on the middle point between two nodes as the configuration shown in Figure 3. In this approach, only local properties of mass, which has to be transferred, need to be recognized without any additional treatment. With this approach, the continuous mass and mass flux are obtained by the LBM without any additional restriction at the interface. This feature will facilitate the modeling of complex problems a great deal.

2.4. Governing Equations for VOC Transportation in Room Air

In order to fully describe the VOC transport process in room air, a complete set of governing equations for VOC transport and room air flow are needed. For Newtonian, incompressible, and laminar flow, the conservation equations for continuity, momentum, and VOC species are as follows.

Continuity equation:

\[
\frac{\partial}{\partial x_j} (\rho u_j) = 0
\]

(20)

![Figure 3. Half-lattice division treatment for the material–material interface.](image-url)
Momentum equation:

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} \left( \rho u_i u_j \right) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} \quad i = 1, 2
\]  

(21)

VOC transport equation:

\[
\frac{\partial}{\partial t} (\rho C) + \frac{\partial}{\partial x_j} (\rho u_j C) = \frac{\partial}{\partial x_j} \left( D_a \frac{\partial C}{\partial x_j} \right)
\]  

(22)

For uniform VOC concentration in the air, which is the assumption of the conventional single-zone approach, the mass balance of VOCs in the air can be given as [4]

\[
\frac{\partial C_a}{\partial t} = N(t) C_{in} - N(t) C_a - LD_y \frac{\partial C(y, t)}{\partial y} \bigg|_{y=b}
\]  

(23)

where \(C_{in}\) is the inlet VOC concentration in the supply air, \(L\) is the material loading factor \([\text{m}^2/\text{m}^3]\) and \(N(t)\) is the air exchange rate \([1/\text{h}]\), whereas the third term on the right side can be obtained through Eq. (12).

In the code developed in this article, the diffusion process in single or multiple solid layers is solved by the LBM, and the air flow and VOC transport in the room are solved by the FVM by discretizing Eqs. (20)–(22). This is what we call the hybrid method. The air flow is assumed to be laminar, and the SIMPLE algorithm is used for solving the flow field. The convection term is discretized by a power-law scheme. When we work at the first step, the above governing equations, i.e., Eqs. (20)–(22), are not solved, and only the transient lumped equation for \(C(y, t)\) is solved numerically. The novelties of our coupled method are in the interface condition treatments mentioned above. Chen et al. coupled the LBM and FVM for many diffusion and fluid flow problems [30, 31]. In their work the exchange of information from both the LBM and FVM zones is necessary, which was done by taking the overlapping zone and using a reconstruction operator. In our study, transfer of information only from solid (LBM) to fluid (FVM) is required, which is achieved by special treatment of the interface lattice, thus eradicating the need for any reconstruction operator or overlapping zone.

3. VALIDATION OF THE PRESENT HYBRID ALGORITHM

The validity of the present hybrid algorithm is ensured by applying it to the following different types of emission processes.

1. First, it is assumed that the concentration of VOCs is totally mixed in the chamber, and the LBM is used for VOC diffusion and emission from material layers in the following emission processes:

   a. VOC emissions in a ventilated chamber: \(N(t) > 0\)
   b. VOC emissions in an airtight chamber: \(N(t) = 0\)
2. Second, the present LBM is coupled with the FVM, as described above, and used to calculate the VOC concentration in the room and is applied to the following cases:

c. VOC emissions in a ventilated room using a single-layer approach

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Dimensions (m)</th>
<th>Pollutant</th>
<th>$C_0$ ($\mu g/m^3$)</th>
<th>$h_m$ (m$^2$/s)</th>
<th>$K_{ma}$</th>
<th>$D_m$ (m$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PB2</td>
<td>0.212 x 0.212 x 0.0159</td>
<td>Hexanal</td>
<td>$2.96 \times 10^7$</td>
<td>$2.5 \times 10^{-3}$</td>
<td>3,289</td>
<td>$7.65 \times 10^{-11}$</td>
</tr>
<tr>
<td>PB2</td>
<td>0.212 x 0.212 x 0.0159</td>
<td>TVOC</td>
<td>$9.86 \times 10^7$</td>
<td>$2.5 \times 10^{-3}$</td>
<td>3,289</td>
<td>$7.65 \times 10^{-11}$</td>
</tr>
<tr>
<td>MDF3</td>
<td>0.1 x 0.1 x 0.0028</td>
<td>Formaldehyde</td>
<td>$1.18 \times 10^7$</td>
<td>$2.5 \times 10^{-3}$</td>
<td>5,400</td>
<td>$4.14 \times 10^{-12}$</td>
</tr>
<tr>
<td>MDF4</td>
<td>0.1 x 0.1 x 0.0028</td>
<td>Formaldehyde</td>
<td>$1.34 \times 10^7$</td>
<td>$2.5 \times 10^{-3}$</td>
<td>5,000</td>
<td>$4.25 \times 10^{-12}$</td>
</tr>
</tbody>
</table>

Figure 4. Comparison of the measured VOC concentration emitted from PB2 in the ventilated chamber: (a) TVOC; (b) hexanal.
d. VOC emissions in a ventilated room with different ventilation positions by using a multilayer approach

3.1. VOC Emission in the Ventilated Chamber

Yang et al. [2] carried out a series of experiments on VOC emissions from particle boards under environmental conditions of 23°C and 50% relative humidity. A 50-L chamber with 1 h⁻¹ air exchange rate was used. The characteristic parameters of hexanal and total VOC (TVOC) for particle board 2 are listed in Table 1. The agreement between the computed results and the experimental data is presented in Figure 4.

The LBM is also used to calculate the VOC emissions from double-layered (porous and nonporous) building materials with a half-lattice division approach. Indoor VOC concentration is analyzed by changing the sequence of the two layers. The baseline parameters are presented in Table 2. The comparison of obtained results with those already published in [32] is presented in Figure 5, showing a very good agreement. The above comparisons indicate suitability of the present LBM with the half-lattice division approach for both sequences of layers.

Table 2. Baseline parameter values of porous and nonporous layers

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume of room</td>
<td>20 m³</td>
</tr>
<tr>
<td>Surface area of VF exposed to air</td>
<td>9 m²</td>
</tr>
<tr>
<td>Flow rate through chamber room</td>
<td>20 m³/h</td>
</tr>
<tr>
<td>Sorption coefficient with porosity</td>
<td>120,000</td>
</tr>
<tr>
<td>Effective diffusivity of porous layer</td>
<td>1.44 × 10⁻⁶ m²/s</td>
</tr>
<tr>
<td>Initial gas-phase concentration of porous layer</td>
<td>1.67 mg/m³</td>
</tr>
<tr>
<td>Thickness of porous layer</td>
<td>0.0002 m</td>
</tr>
<tr>
<td>Partition coefficient of nonporous layer</td>
<td>120,000</td>
</tr>
<tr>
<td>Diffusion coefficient of nonporous layer</td>
<td>1.2 × 10⁻¹³ m²/s</td>
</tr>
<tr>
<td>Initial concentration of nonporous layer</td>
<td>200 g/m³</td>
</tr>
<tr>
<td>Thickness of nonporous layer</td>
<td>0.0018 m</td>
</tr>
</tbody>
</table>

Figure 5. Comparison of the simulated results for both sequences of layers.
As in most cases, ventilation rate is not constant, the present LBM is used to analyze the effect of ventilation rate on the concentration of VOCs. The sinusoidal variation pattern of ventilation is considered here:

\[ N(t) = 0.9 \sin \left( \frac{\pi}{4} (t + 2) \right) + 1.1 \]  \hspace{1cm} (24)

where \( t \) is the time in hours.

Figure 6 shows that the variation pattern of gas-phase VOC concentration in air, for both sequences of porous/nonporous layers, is similar to that of the air exchange rate \( N(t) \). On the other hand, the concentration decreases with time in both

![Figure 6. VOC concentration in air for sinusoidal ventilation: (a) top nonporous layer, bottom porous layer; (b) top porous layer, bottom nonporous layer.](image-url)
cases. These results show that, at least qualitatively, the VOC concentration variation pattern is correct.

In order to further evaluate the validity of the present lattice Boltzmann method, it is employed to calculate the VOC concentration in a room where floor carpet is an emitting source of VOCs and the walls and roof are exhibiting source/sink behavior. Moreover, all the materials taken into account are composed of multiple porous layers. As Figure 7 presents, the computed concentrations accord well with those given by Zhang and Niu [7], where all characteristic parameters used in the simulation can be found.

3.2. VOC Emission in the Airtight Chamber

The present LBM is now employed for calculation of VOCs in an airtight chamber (air exchange rate being zero), which, to the best of authors’ knowledge, has never been simulated before. The simulated results are compared with experimental results obtained by Wang and Zhang [12]. The characteristic parameters of formaldehyde for MDF3 and MDF4 are listed in Table 1. Figure 8 shows a reasonable conformity between the simulated results and the experimental data.

3.3. VOC Emission in a Ventilated Room with Different Ventilation Positions

After checking the accuracy of the LBM by applying it to various types of VOC emission processes with the single-zone model shown above, it is coupled with the FVM to study the VOC distribution in a ventilated room using both single- and multilayer approaches.

3.3.1. Single layer approach. The 2-D room model (4.5 m × 3.0 m) shown in Figure 9 as proposed by Murakami et al. [33] is used as a benchmark. The

![Figure 7. Comparison of predicted indoor ethyl acetate concentration.](image)
polypropylene styrene-butadiene rubber (SBR) plate is used as a VOC source. The initial VOC concentration distribution in the SBR is assumed to be uniform, $C_0 = 1.92 \times 10^8 \text{mg/m}^3$, with effective diffusion coefficient $D_s = 1.1 \times 10^{-14} \text{m}^2/\text{s}$ at $23^\circ \text{C}$. The inflow velocity is $0.1 \text{m/s}$ with air exchange rate $1.6 \text{h}^{-1}$. As indicated above, the lattice surface point $n$ in Figure 9 should be specially treated, i.e., the surface lattice is taken as a normal lattice but with different diffusivities, whereas the exchange of information between the surface lattice and other lattices is handled through a half-lattice division approach.

### 3.3.2. Multilayer approach.

Consider the same room with the same dimensions as in the single-layer case but with a floor composed of three layers of different materials, from bottommost layer to uppermost layer, 200 mm concrete, 10 mm gypsum board, and 15 mm carpet, as shown in Figure 10 [7]. Ethyl acetate is selected...
as a VOC source found only in carpet. This compound evaporates easily at room temperature because of its low boiling point, and its vapors are readily inhaled by occupants in the room. The chemical and physical properties of ethyl acetate are

<table>
<thead>
<tr>
<th>VOC properties</th>
<th>Ethyl acetate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular formula</td>
<td>CH₃COOC₂H₅</td>
</tr>
<tr>
<td>Molecular weight (g mol⁻¹)</td>
<td>88.1</td>
</tr>
<tr>
<td>Boiling point (°C)</td>
<td>77.1</td>
</tr>
<tr>
<td>Polarity (10⁻²⁴ m³)</td>
<td>9.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Material</th>
<th>Effective diffusivity (m²/s)</th>
<th>Sorption coefficient (m³ air/m³ material)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carpet with SBR backing</td>
<td>4.52 × 10⁻⁷</td>
<td>42.2</td>
</tr>
<tr>
<td>Solid concrete</td>
<td>5.06 × 10⁻⁸</td>
<td>1,140.69</td>
</tr>
<tr>
<td>Gypsum board</td>
<td>1.13 × 10⁻⁶</td>
<td>86.65</td>
</tr>
</tbody>
</table>
listed in Table 3. The effective diffusion and sorption coefficients of selected materials employed here have been measured by Meininghaus et al. [34] and are listed in Table 4, whereas density and porosity of selected materials are listed in Table 5. All calculations are performed at 23°C with inlet velocity 0.2 m/s for a maximum time of 50 h. The initial gas-phase concentration of ethyl acetate in the carpet is taken to be 236.97 mg/m³ [7].

4. RESULTS AND DISCUSSION FOR LBM-FVM COUPLED SIMULATION

A typical 2-D room with dimensions 4.5 m × 3.0 m is considered as benchmark. The room average VOC concentration as shown in Figure 11 is computed by using the hybrid algorithm, and it is found that results are in very good agreement with those already published [33]. As shown in Figure 12, it is also found that, with the given inlet outlet positions, the maximum normalized value of VOC concentration is 8.99E⁻⁸. The same room with a floor composed of three different materials, in which only carpet has a VOC source, has been simulated by the proposed hybrid algorithm to find the best inlet/outlet position for the breathing zone of sitting/standing people. The results of VOC concentration distribution for four combinations of inlet/outlet are presented in Figure 13. Figure 13b shows the best combination of inlet and outlet for the room, in which most of the room area has the least VOC concentration in the breathing zone of sitting/standing people, as compared to three other ventilation organizations, if sitting and standing near the left wall is avoided (where VOC concentration is abundant).

<table>
<thead>
<tr>
<th>Material</th>
<th>Density</th>
<th>Porosity (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carpet with SBR backing</td>
<td>1,300</td>
<td>10</td>
</tr>
<tr>
<td>Solid concrete</td>
<td>295.29</td>
<td>15</td>
</tr>
<tr>
<td>Gypsum board</td>
<td>774.4</td>
<td>28</td>
</tr>
</tbody>
</table>

Figure 11. Profile of room-averaged concentrations with time.
5. CONCLUSION

In this article the hybrid algorithm, coupled FVM and LBM, for VOC emission has been presented. The LBM has been employed for VOC diffusion through materials comprised of single as well as multiple porous and nonporous layers, and the FVM has been adopted for the flow and transport of VOCs in the room with the interface conditions being carefully treated. In the multilayer situation, the LBM half-lattice division approach has been employed, and the benchmark results confirm the feasibility of this approach. The good agreement between experimental data and numerical results for VOC emission in an airtight chamber increases the validity.
range of the present LBM. The effect of both sequences of porous/nonporous layers and variable air exchange rate has also been studied. At the interface between different material layers, with the half-lattice division approach, just local properties of mass being diffused need to be considered, without any additional treatment. The current algorithm has also been used for numerically calculating the distribution of VOC concentration in the room, and the best ventilation organization for breathing zones of sitting/standing people in the room is found.

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REFERENCES


