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Indoor Diffusion Model of Volatile Organic Compounds in Building Materials Based on Cloud Computing

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Based on the cloud computing platform, this paper constructs an analytical model for the indoor diffusion process of volatile organic compounds (VOCs) in building decoration materials. The model considers key parameters such as diffusion concentration, diffusion coefficient, and closed chamber background value, and validates the model through practical examples. The results show that the VOC diffusion law obtained by the proposed model and the numerical simulation calculation model is basically the same, and the calculation time of the proposed model is shorter. The VOCs in indoor building materials mainly undergo two stages of diffusion mass transfer and convective mass transfer, and finally diffuse into the space of the closed chamber. In the early and middle stages of VOC diffusion, the environmental concentration in the closed chamber changes drastically. In the late stage of diffusion, in the closed chamber, the environmental concentration gradually reaches equilibrium, and the mass transfer characteristics of the VOC are basically unaffected by the area of the closed chamber and the air flow rate.

1. Introduction

About 80% of a person's life is working and living indoors. The high quality of indoor air is a prerequisite for human health. In recent years, relevant research has shown that excessive indoor building material VOCs is an important reason causing symptoms such as lack of energy, fatigue, and nausea. Long-term living in an environment containing VOCs such as benzene, formaldehyde will greatly increase the probability of cancer in the human body (Xiong et al., 2013; Wang et al., 2013; Klepeis et al., 2001; Zhang and Ying, 2003). Studying the diffusion law of indoor building materials is important for improving indoor air quality and ensuring human health (Li, 2013; Howard-Reed et al, 2011; Hammond et al., 2018).

The VOC diffusion process simulation method has the advantages of low cost, short test period, and various considerable complicated conditions. It has become the main method for the research and prevention of the diffusion law of VOCs (Xu and Zhang, 2004; Xiong et al., 2011; Grysakowski, 2016). The existing models are mainly divided into two categories: empirical models and theoretical models. The empirical model is established according to a large amount of data from on-site monitoring, and it has large limitations (Liu et al, 2015); the core of the theoretical model is the mass transfer equation (Seelam, 2018; Balocco and Petrone, 2018; Zhang and Li, 2008; Hu et al, 2007; Wang and Zhang, 2011), mainly including building material VOC diffusion analytical model, semi-analytical model, approximate integral numerical algorithm, etc. (Deng and Chang, 2004; Ye et al., 2017; Choi, 2015). Compared with the empirical model, the calculation result of the theoretical model is closer to reality, but there are also idealized practices such as ignoring the convective mass transfer resistance and assuming that the initial VOC concentration is zero (Xu and Zhang, 2003). At the same time, all the above theoretical models did not consider the actual diffusion law of VOC under the interaction of key parameters such as diffusion concentration and diffusion coefficient in VOC diffusion process (Crawford and Lungu, 2013; Hussain et al, 2015).

The theoretical analytical model in this paper considered key parameters such as diffusion concentration, diffusion coefficient and background value of the closed chamber. Based on the cloud computing platform, the model proposed in this paper is verified by practical examples.

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2. Construction of theoretical analytical model for VOC diffusion process

Figure 1 shows a schematic diagram of the diffusion of building material VOCs in a closed chamber. The governing equation for the diffusion of building material VOCs indoors can be expressed as Eq (1).

$$\frac{\partial C_{\mathrm{m}}}{\partial t}=D\frac{\partial^2 C_{\mathrm{m}}}{\partial x^2},C_{\mathrm{m}}\big|_{t=0}=C_0 \tag{1}$$

C_m is the concentration of building material VOCs at the initial moment; t is the calculation time. When the VOCs are easily to flow or adsorbed by indoor walls, the boundary condition is shown in Eq (2).

$$\left.\frac{\partial C_{\mathrm{m}}}{\partial x}\right|_{x=0}=0,-D\left.\frac{\partial C_{\mathrm{m}}}{\partial x}\right|_{x=L}=h_{\mathrm{m}}\left(\frac{C_{\mathrm{m}}\big|_{x=L}}{K}-C_{\mathrm{a}}\right) \tag{2}$$

The mass balance equation in a closed chamber is shown in Eq (3).

$$V\frac{\mathrm{d}C_{\mathrm{a}}}{\mathrm{d}t}=-AD\left.\frac{\partial C_{\mathrm{m}}}{\partial x}\right|_{x=L},C_{\mathrm{a}}\big|_{t=0}=C_{\mathrm{b}} \tag{3}$$

D is the diffusion coefficient of the indoor VOC. L is the thickness of the building material. K is the distribution coefficient. C_a is the concentration of the indoor VOC after the elapse of time t. C_b is the background value of the closed chamber.
Transform Eq (1) to (3) to obtain full analytical solutions of C_a and C_m as Eq (4) and (5).

$$C_{\mathrm{a}}=\frac{C_0\beta+C_{\mathrm{b}}}{K\beta+1}+2\sum_{n=1}^{\infty}\frac{\left(C_0\beta-q_n^2C_{\mathrm{b}}KBi_{\mathrm{m}}^{-1}\right)\sin q_n+q_nC_{\mathrm{b}}\cos q_n}{q_nA_n}\times\mathrm{e}^{-\frac{Dq_n^2}{L^2}t} \tag{4}$$

$$C_{\mathrm{m}}=\frac{C_0K\beta+KC_{\mathrm{b}}}{K\beta+1}+2\sum_{n=1}^{\infty}\frac{C_0K_n-q_n\left(C_0-KC_{\mathrm{b}}\right)\cos\left(\frac{x}{L}q_n\right)}{q_nA_n}\times\mathrm{e}^{-\frac{Dq_n^2}{L^2}t} \tag{5}$$

After the time t, the VOC concentration in the closed chamber reaches equilibrium, and the indoor air balance concentration $C_{a,\,equ}$ and the equilibrium concentration $C_{m,\,equ}$ of the VOCs are shown in Eq (6):

$$C_{\mathrm{a,equ}}=\frac{C_0\beta+C_{\mathrm{b}}}{K\beta+1},C_{\mathrm{m,equ}}=K\frac{C_0\beta+C_{\mathrm{b}}}{K\beta+1} \tag{6}$$

Using Eq (5), the diffusion rate R_a and the diffusion amount M of the building material VOCs can be obtained as Eq (7) and (8):

$$R_{\mathrm{a}}=-D\left.\frac{\partial C_{\mathrm{m}}}{\partial x}\right|_{x=L}=-\frac{2D\left(C_0-KC_{\mathrm{b}}\right)}{L}\sum_{n=1}^{\infty}\frac{q_n\sin q_n}{A_n}\times\mathrm{e}^{-\frac{Dq_n^2}{L^2}t} \tag{7}$$

$$M=\int_0^t R_{\mathrm{a}}\mathrm{d}\tau=2L\left(C_0-KC_{\mathrm{b}}\right)\sum_{n=1}^{\infty}\frac{\sin q_n}{q_nA_n}\times\left(\mathrm{e}^{-\frac{Dq_n^2}{L^2}t}-1\right) \tag{8}$$

3. Influence of background value of closed chamber C_b on VOC diffusion process

Convert Eq (4) to Eq (9).

$$C_{\mathrm{a}}^*=\frac{K\beta+C_{\mathrm{b}}^*}{K\beta+1}+2\sum_{n=1}^{\infty}\frac{K\beta\sin q_n+B_{\mathrm{a}}C_{\mathrm{b}}^*}{q_nA_n}\times\mathrm{e}^{-Fo_mq_n^2} \tag{9}$$

According to Eq (9), the change of VOC concentration in the closed chamber under different C_b values can be calculated.

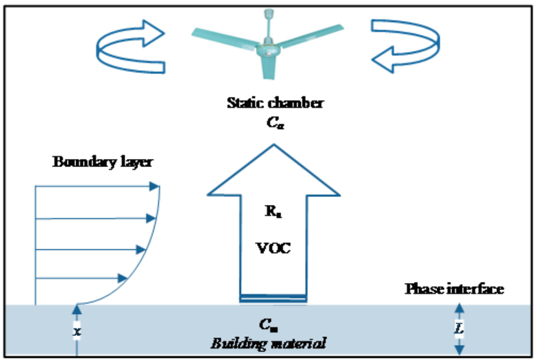


Figure 1: Schematic diagram of VOC diffusion

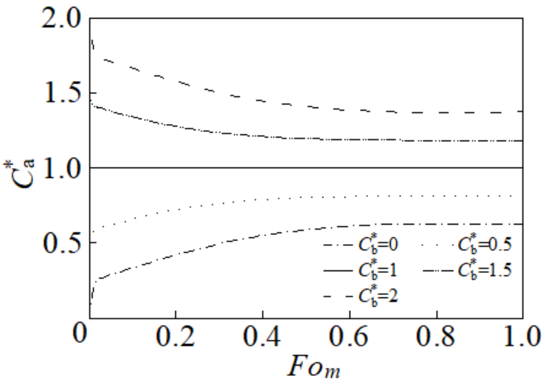


Figure 2: Changes in VOC concentration

It can be seen from the figure 2 that when C_b<1, the indoor VOCs are in a divergent status as a whole, at which time the VOCs diffuse from the building material into the room, and when C_b gradually approaches 1, the C_b basically approaches a certain value, and the indoor equilibrium concentration is higher;
When C_b=1, the closed chamber VOCs are almost in a constant status;
When C_b>1, the indoor VOCs are in an adsorbed status as a whole, at which time the VOCs migrate from the closed chamber into the building material, and when C_b approaches 1, the indoor equilibrium concentration is lower.
From the above analysis we can know that, the critical value of VOC diffusion or adsorption is C_b=1, the critical background value is set as $C_{b,\,c}$, and there is C_b<$C_{b,\,c}$, $C_{b,\,c}$=C_0/K.
Convert the $C_{a,\,equ}$ expression to Eq (10):

$$C_{a,equ}=\frac{C_0\beta+C_b}{K\beta}\times\frac{K\beta}{K\beta+1}=\frac{C_0\beta+C_b}{K\beta}r=r\left(\frac{C_0}{K}+\frac{C_b}{K\beta}\right)=r\left(C_{b,c}+\frac{C_bR}{K}\right)\tag{10}$$

According to Eq (10), there is $C_{a,\,equ}$ = $C_{b,\,c}$ under a certain condition.

4. Test results and analysis

Taking the typical VOCs contained in five kinds of building materials commonly used in interior decoration (furniture, floor, ceiling, medium density fiberboard (MDF), joinery board) as an example, the mass transfer parameters are introduced into the theoretical model established in this paper, and the calculation results are compared with Huang, Xu and numerical calculation model. The prediction results of the model in this paper and the calculation results of other models are shown in Figure 3(a) and Figure 3(b), respectively.

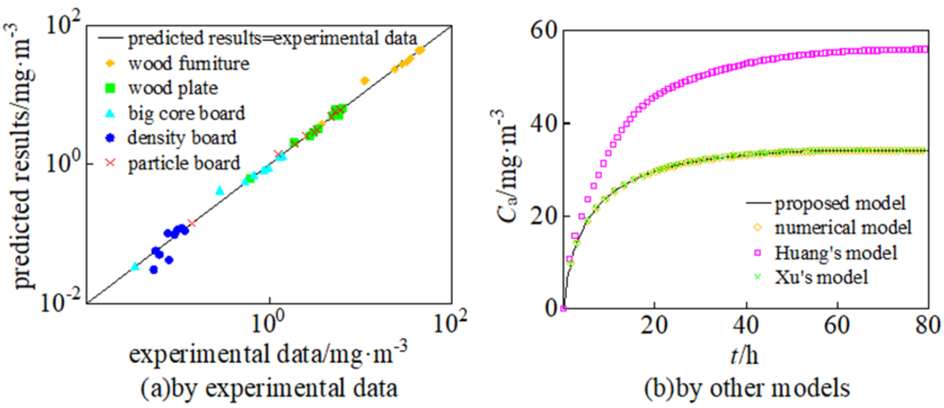
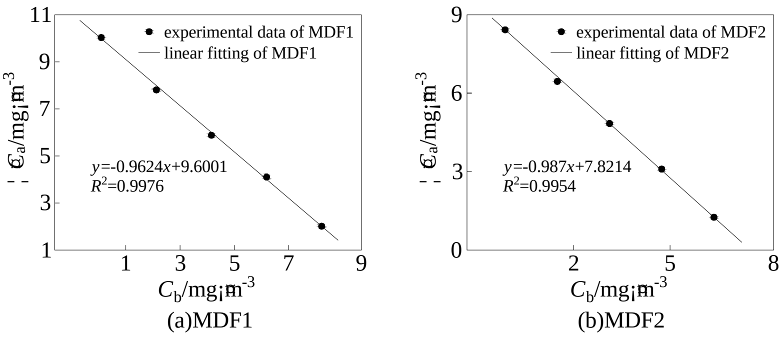


Figure 3: Model prediction results

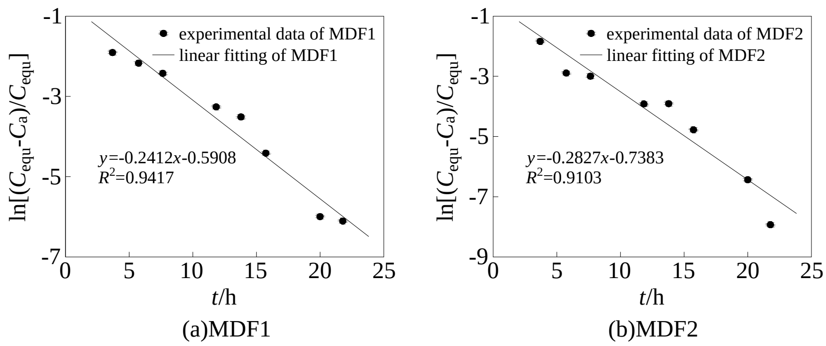
It can be seen from the figure that the VOC diffusion process of the Huang model is higher than other models, because the Huang model does not consider the environmental concentration change in the closed chamber during the calculation process; while in the Xu model, the numerical simulation calculation model and the proposed theoretical model, the VOC diffusion law is basically the same.

As shown in figure 4 to 6, the calculation results of four mass transfer parameters (C_0, K, D and h_m) in a closed chamber. In this paper, two sets of calculation parameters are adopted, namely MDF1 and MDF2. It can be seen from the figure that the fitting value correlation coefficients R^2 of the four parameters are all above 0.9, which satisfies the requirement of R^2>0.81, it indicates that the indoor VOC calculation accuracy of the theoretical model proposed in this paper is higher. It can be seen that the time required to reach the VOC concentration equilibrium in the closed chamber is inversely proportional to the C_b value, that is, the larger the C_b value. It takes the shorter time to reach the balance, and the relevant calculation results show that the proposed model can calculate 4 kinds of mass transfer parameter values that meet the requirement within 4d, while the traditional algorithm needs about 1 month.



(a) C_0 *(b) K*

Figure 4: Calculation results of C0 and K values



(a) D *(b) h_m*

Figure 5: Calculation results of D and hm values

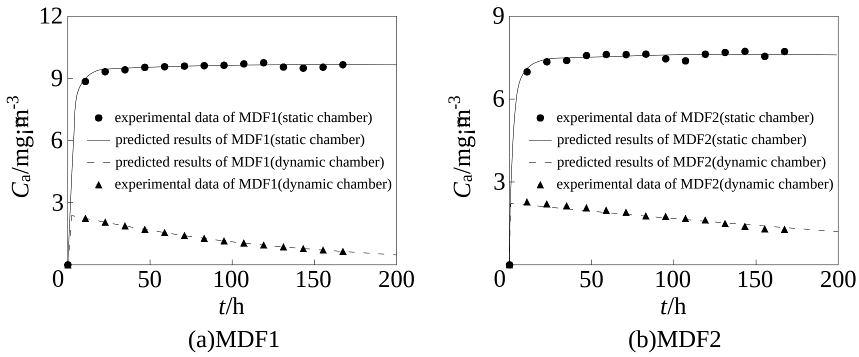


Figure 6: Comparison of test results and fitting results

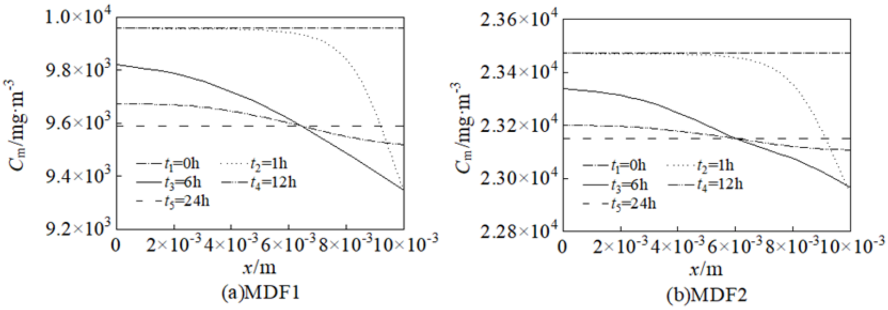


Figure 7: Diffusion of building material VOCs at different distances under various test times

Figure 7 shows the diffusion of building material VOCs at different distances for the two sets of mass transfer parameters. It can be seen from the figure that the VOC concentrations in the closed chamber of the two mass transfer parameters reach equilibrium at around 24 h, and the environmental C_a standard deviations in the closed chamber are 3.8% and 1.6%, respectively, all of which are less than the judging criterion that the standard deviation of the closed chamber is less than 5%. As the C_b value increases, the environmental C_a standard deviation is smaller when the VOC concentration in the closed chamber reaches equilibrium.

The concentration of VOCs in the building material decreased from a steady decline to a rapid decline, and finally began to decline steadily. The equilibrium of the closed chamber satisfies the requirements at all times.

The VOCs in building materials mainly undergo two stages of diffusion mass transfer and convective mass transfer, and finally diffuse into the closed chamber. In the early and middle stages of VOC diffusion, the environmental concentration in the closed chamber changes drastically; in the later stage of diffusion, the environmental concentration in the closed chamber gradually reaches the equilibrium state.

5. Conclusion

In this paper, a theoretical analytical model for the diffusion process of VOCs in building decoration materials is established. The model considers the key parameters such as diffusion concentration, diffusion coefficient and diffusion distance, and validates the model proposed in this paper through practical examples. The research conclusions are as follows:

(1) The actual example verification results show that the VOC diffusion law obtained by the model and the numerical simulation model is basically the same, and the calculation time of the proposed model is shorter, which proves the feasibility and superiority of the proposed algorithm.

(2) Using the algorithm of this paper, the parameters such as VOC diffusion coefficient and mass transfer coefficient can be accurately obtained, and the equilibrium concentration in the closed chamber and the time taken to reach the equilibrium state can be obtained. The VOCs in building materials mainly undergo two stages of diffusion mass transfer and convective mass transfer, and finally diffuse into the closed chamber. In the early and middle stages of VOC diffusion, the environmental concentration in the closed chamber changes drastically; in the later stage of diffusion, the environmental concentration in the closed chamber gradually reaches equilibrium, at this time the mass transfer characteristics of VOC are basically not affected by the area of the closed chamber and the air flow rate.

(3) The diffusion process of VOCs is affected by many reasons: indoor temperature and humidity stability; multi-dimensional non-uniform diffusion and cross-diffusion of various VOCs. In the subsequent research, the detection and analysis dimensions of the organic matter diffusion process will be increased, and an analytical model closer to the actual situation will be established to provide a basis for selecting proper absorber, photocatalytic equipment and determining the ventilation volume.

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