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Numerical simulation of VOCs emission from building materials: A comparison of different material shapes

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ABSTRACT

Introduction: Volatile Organic Compounds (VOCs) are the most significant indoor pollutants that mainly emitted from various building materials and can do a great harm to human beings. The present study aims to the effect of different shapes of building materials on the emission characteristics of VOCs by using Computational Fluid Dynamics (CFD) simulation.

Materials and methods: The indoor air flow is described by the continuity equation, the momentum equation and the standard k-ε model. The transport of VOCs in materials is described by a transient diffusion equation. ANSYS Fluent is used to solve the governing equations.

Results: The emission of VOCs from planar building materials is validated based on the experimental data according to the literature. The numerical results have proved that the emission VOCs from hollow cylindrical building materials is faster than that of VOCs from planar building materials. The thinner the building materials and diffusion coefficient is bigger, the faster decrease rate of VOCs it is.

Conclusion: The material shape has a significant impact on the emission of VOCs from building materials. When assessing indoor air quality, the realistic shape of materials should be used instead of the simplified planar materials.

Introduction

In most of modern buildings, many materials such as tiles, carpets, paints and wood products are widely used to decorate the indoor environment. These materials can release a large amount of pollutants, mainly including alcohols, hydrocarbons and amines and Volatile Organic Compounds (VOCs) [1–3]. VOCs are the most hazardous pollutants in the indoor environment and can cause sick building syndrome, building related illness and multiple chemical sensitivity [4–7]. Most indoor VOCs are emitted from indoor building materials [8, 9]. Therefore, it is essential to investigate the emission characteristics of VOCs from building materials in order to provide theoretical guidance for improving indoor air quality.

Many experimental studies were conducted to measure the emission of VOCs from building materials [1, 10–18]. A rectangular material

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with a small thickness was usually placed in an environmental test chamber. VOCs were emitted through a planar surface into the air. The concentrations of VOCs in the test chamber was measured at intervals. Many researchers, firstly modelled the emission of VOCs from a carpet in the environmental test chamber using the Fickian diffusion [19]. The initial concentration of VOCs in building materials, the partition coefficient at the material-air interface, and diffusion coefficient of VOCs in building materials were thought to the key parameters describing the transport of VOCs within the building material. Subsequently, the diffusion-based emission model has been improved by many workers to consider the mass transfer resistance in the boundary layer [20–23], the emission of VOCs in multi-layer materials [24–28] and the emission of SVOCs [29–31]. Although those models have been very successful in the simulation of VOCs emission from building materials, they virtually only considered the emission of VOCs from a planar surface.

Other researchers developed a method to measure gas-phase SVOC concentration near material surface [32]. A cylindrical thermal desorption tube was used to adsorb VOCs emitted from the material. A 2D numerical simulation was performed to study the emission of VOCs in the cylindrical coordinate. To the best of the authors' knowledge, no study has yet focused on the emission of VOCs from the cylindrical surface. In the present study, the emission of VOCs form hollow cylindrical materials is considered using a three-dimensional CFD model and the diffusion-based emission model. The effect of diffusion coefficient and the thickness of the material on the emission from hollow cylindrical materials and planar materials are discussed in detail.

Materials and methods

Geometry

Many volatile organic compounds can be emitted from building materials. Total Volatile Organic Compound (TVOC) is often used to rank building materials. In a study it was found that major compounds were emitted from a particleboard [33]. The concentration of TVOC, Hexanal and α. Pinene were measured. Herein, the emissions of TVOC from hollow cylindrical and planar particleboard are investigated. The particleboard can emit hexanal and α. pinene. The surface of planar material has dimensions of 10 cm×3 cm. The hollow cylindrical material has an outer diameter of 3.2 cm and a height of 2.986 cm. It is assumed that TVOC is emitted only from the upper surface of the planar material and the outer cylindrical surface of the hollow cylindrical material. Thus, both materials have the same surface area of 30 cm^2 to emit TVOC. The emissions from both materials are simulated in a test chamber having dimensions of 50 cm×40 cm×25 cm, as shown in Fig. 1

Governing equations

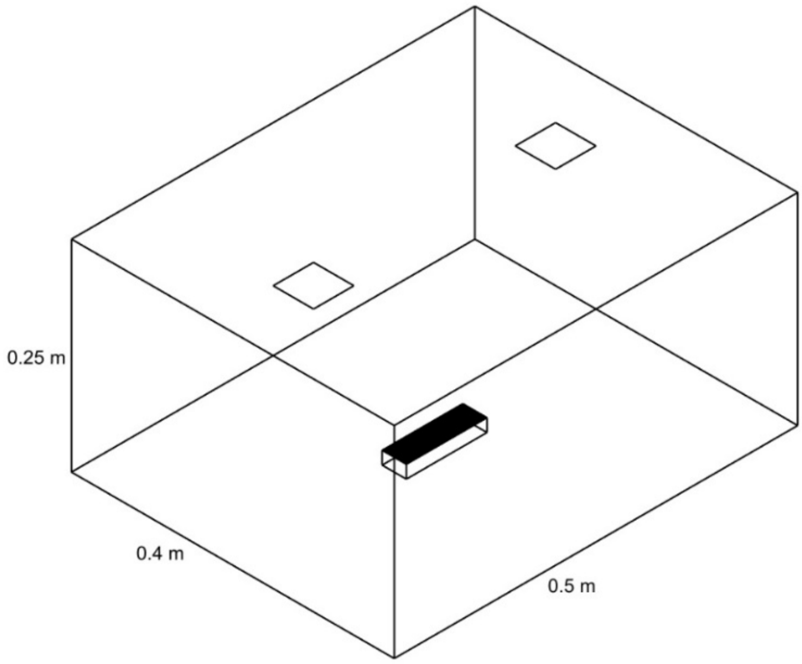
The airflow in the test chamber has a strong influence on the emission of TVOC from building materials. It is assumed that the flow in the test chamber is incompressible and steady. The continuity equations and the momentum equation can be described as follows:

$$\frac{\partial}{\partial x_j}\left(\rho u_j\right) = 0 \tag{1}$$

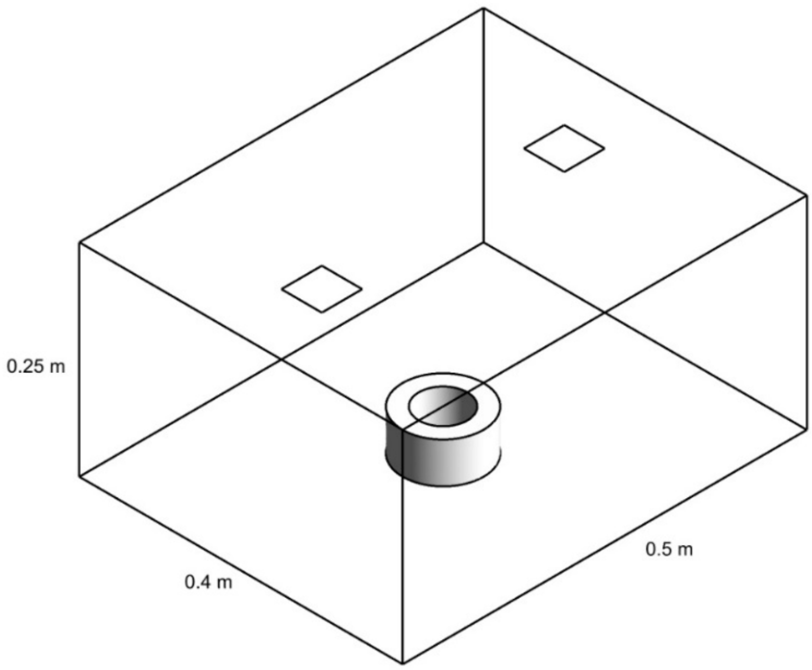
$$\frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = \frac{-\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}\left\{\rho(v + v_t)\frac{\partial u_i}{\partial x_j}\right\} \tag{2}$$

$$v_t = C_\mu \frac{k^2}{\varepsilon} \tag{3}$$

Where ν is the laminar kinematic viscosity, ν_t is the turbulent kinematic viscosity, u_i and u_j are the velocity components in the i and j directions, respectively, k is turbulent kinetic energy, ε is turbulence dissipation rate. The turbulent kinematic viscosity is solved using the standard k-ε model as follows:



(a) planar material



(b) hollow cylindrical material

Fig. 1. Schematic of geometric of building materials

$$\frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j}[\rho(v + v_t/\sigma_k)] + G_k - \rho\varepsilon \quad (4)$$

$$\frac{\partial}{\partial x_j}(\rho u_j \varepsilon) = \frac{\partial}{\partial x_j}\left[\rho(v + v_t/\sigma_\varepsilon)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{\varepsilon 1}\frac{\varepsilon}{k}G_k - C_{\varepsilon 2}\frac{\rho\varepsilon^2}{k} \quad (5)$$

Where G_k is the generation of turbulent kinetic energy. The model constants were calibrated to be:

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

TVOC is emitted from building materials and go into the air. Thus, the transport of TVOC in the air and build materials need to be considered simultaneously. The distribution of TVOC concentration in the air is described by the convection diffusion equation.

$$\frac{\partial C_a}{\partial \tau} + \frac{\partial (u_j C_a)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\frac{v}{Sc} + \frac{v_t}{Sc_t}\right)\frac{\partial C_a}{\partial x_j}\right) \quad (7)$$

Where C_a is the equivalent TVOC concentration. As described in the section 2.1, both the planar material and the hollow cylindrical material are considered. The transport of TVOC in building materials is simulated by using the Fickian second Law, as follows

$$\frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial y^2} for 0 < y < \delta \quad (8)$$

for the planar material, and

$$\frac{\partial C_m}{\partial t} = \frac{D_m}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_m}{\partial r}\right) for r_1 < r < r_2 \quad (9)$$

For the hollow cylindrical material, where C_m is TVOC concentration in building materials, D_m is the diffusion coefficient of TVOC in building materials, t is time, y is the coordinate along the thickness of planar building materials, and r is radial coordinate of hollow cylindrical building materials.

At the initial time, TVOC is assumed uniform within the material, as follows

$$C_m|_{t=0} = C_0 \quad (10)$$

It is assumed that TVOC can be emitted only from the upper surface of the planar material and the outer cylindrical surface of the hollow cylindrical material. Therefore, at the bottom of the planar material and the inner cylindrical surface of hollow material, no TVOC can be released, which means

$$\left.\frac{\partial C_m}{\partial x}\right|_{x=0} = 0 \quad (11)$$

and

$$\left.\frac{\partial C_m}{\partial r}\right|_{r=r_1} = 0 \quad (12)$$

At the emitting interface, a linear equilibrium is assumed between the air phase concentration and the material phase concentration and no TVOC can accumulate, which reads

$$\begin{cases} C_m|_{x=\delta} = K_{ma}C_a \\ -D_m\left.\frac{\partial C_m}{\partial x}\right|_{x=\delta} = -\left(\frac{v}{Sc} + \frac{v_t}{Sc_t}\right)\left.\frac{\partial C_a}{\partial x}\right|_{x=\delta} \end{cases} \quad (13)$$

and

$$\begin{cases} C_m|_{r=r_2} = K_{ma}C_a \\ -D_m\left.\frac{\partial C_m}{\partial r}\right|_{r=r_2} = -\left(\frac{v}{Sc} + \frac{v_t}{Sc_t}\right)\left.\frac{\partial C_a}{\partial r}\right|_{r=r_2} \end{cases} \quad (14)$$

Simulation detail

As pointed out by researchers, the diffusion of TVOC in building materials can be categorized into single-phase model and porous medium model [34]. Herein the single-phase model is used to describe the diffusion of TVOC in building materials. CFD model is used to solve the concentration in the air. The computational domain is discretized using the tetrahedral grid with 432648 and 931382 cells for the planar and hollow cylindrical building materials, respectively. Here a particle board and TVOC are selected for research.

The diffusion coefficient, TVOC initial concentration and the partition coefficient of building materials are 7.65×10^{-11} m^2/s, 5.28×10^{7} $\mu g/m^3$ and 3289, respectively. The inlet velocity, turbulence intensity and turbulence length scale are set to be 0.0303 m/ s, 10% and 0.212 m, respectively. No-slip conditions are adopted at all walls. The concentration of TVOC at the inlet is zero. A pressure outlet is set at the outlet. The gradients of TVOC concentration at all walls are zero.

The finite volume method is used to discretize all governing equations. ANSYS Fluent is used to solve the discretized equations. The SIMPLE algorithm is used to treat the pressure-velocity coupling. The second-order upwind scheme and the central difference scheme are adopted to discretize the convective terms and diffusion terms, respectively. The flow equations are assumed to converge when residuals are less than 1.0×10^{-4}. After obtaining the flow field, the TVOC concentration is solved in an unsteady manner with a time step of 60 s.

Results and discussion

Validation of the numerical model

The numerical model of TVOC emission from planar building materials was verified by using the experiment data reported by a study [33]. A particleboard having dimensions 21.2 cm×21.2 cm×1.59 cm was placed in the test chamber shown in Fig . 1. The air exchange rate was 1/ h. The initial TVOC concentration in particleboard is assumed to be 5.28×10^{7} $\mu g/m^3$. Fig. 2 shows the volume-averaged TVOC concentration in the air. The TVOC concentration increases sharply and then decreases slowly. The TVOC concentrations for the experiment and present simulation reach peak values almost at the same time. The present results are in good accordance with the experimental data, indicating that the present numerical model is capable of predicting the emission of TVOC from building materials.

The volume-averaged concentration of TVOC

Fig. 3 shows the volume-averaged concentration of TVOC in the air for two kinds of materials. Both plots have the same tendency when time proceeds. The volume-averaged TVOC concentrations in the air rise sharply to the peaks and then decrease slowly to a pseudo dynamic equilibrium due to the nearly the same values of the TVOC emission rate and the depletion at the outlet. However, the peak values of those two materials show an obvious difference. The maximum concentration of TVOC for the hollow cylindrical building materials is higher than that for the planar building materials, indicating that the emission of TVOC from the hollow cylindrical building material is faster than that from the planar building material.

The effect of material thickness

Figs. 4-6 illustrate the effect of the material thickness on the volume-averaged concentration in materials. When the material thickness is 0.5 cm, the non-dimensional concentration approaches zero after 5 to 8 days. However, the non-dimensional concentration in the hollow cylindrical material decays faster than that in the planar material. When the material thickness increases to 1 cm, the non-dimensional concentration approaches zero at 20 days for the hollow cylindrical material, whereas at 30 days for the planar material. This tendency is further enhanced when the material thickness increases to 1.5 cm. It means that the material thickness plays an important role in the emission of TVOC for planar and hollow cylindrical materials. When the material thickness is relatively big compared to the cylinder diameter, the simplification of hollow cylindrical material to planar material may lead to a large error in the first days of emission.

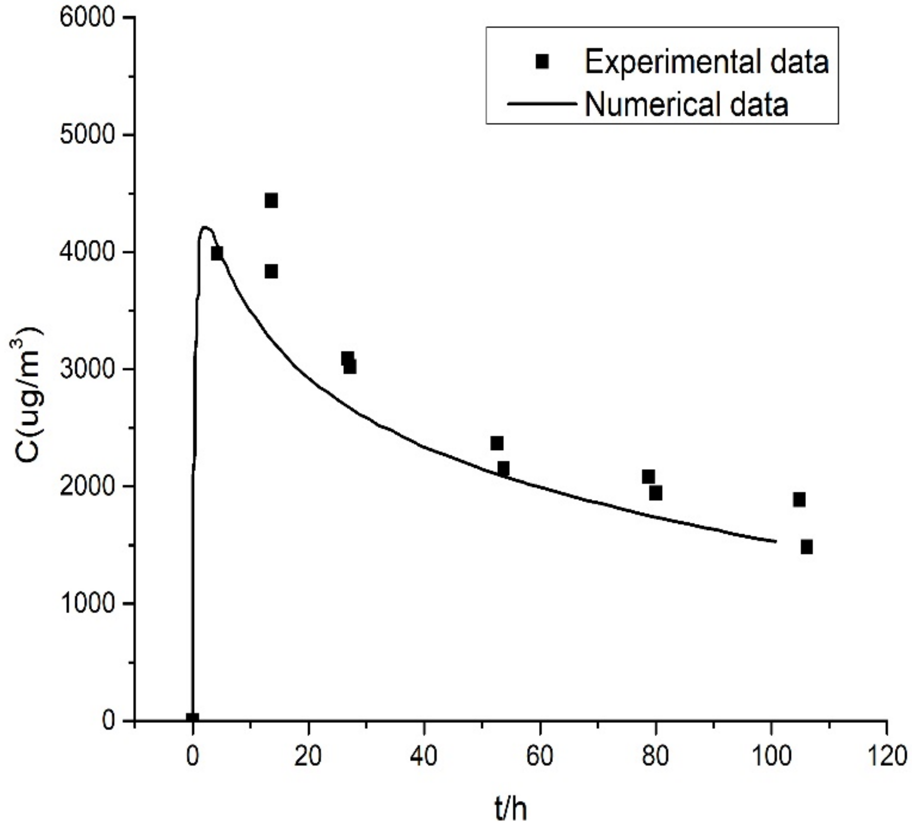


Fig. 2. Validation of the computed TVOC concentrations and the experimental data

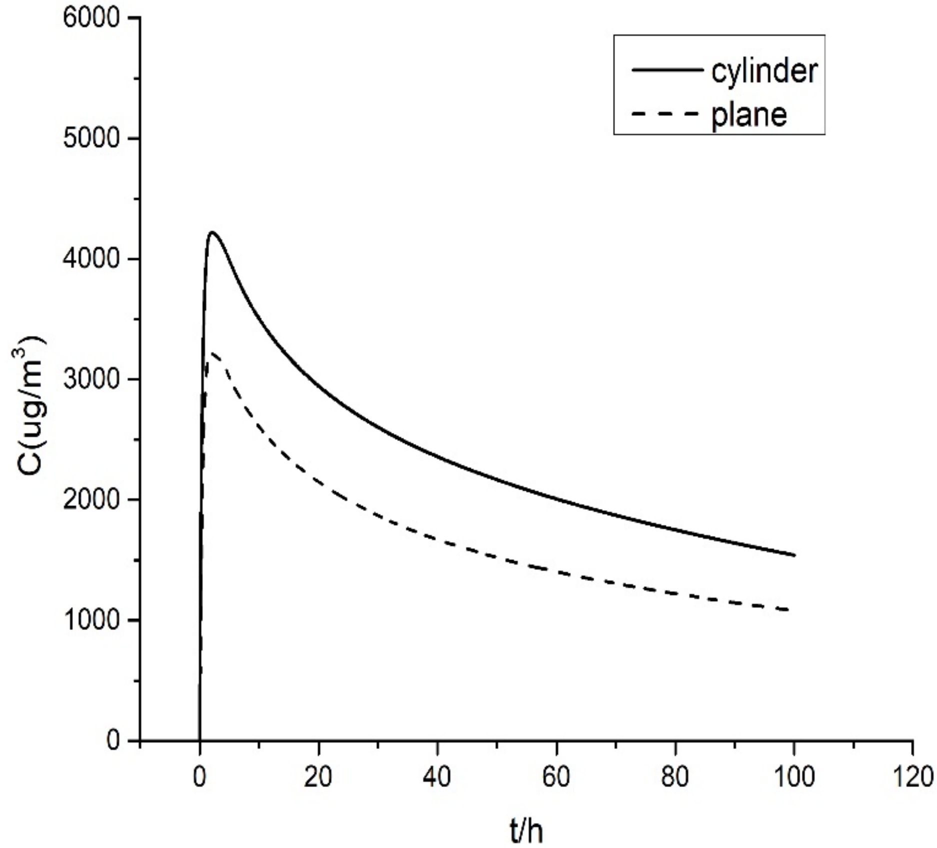


Fig. 3. The volume-averaged concentration of TVOC in the air

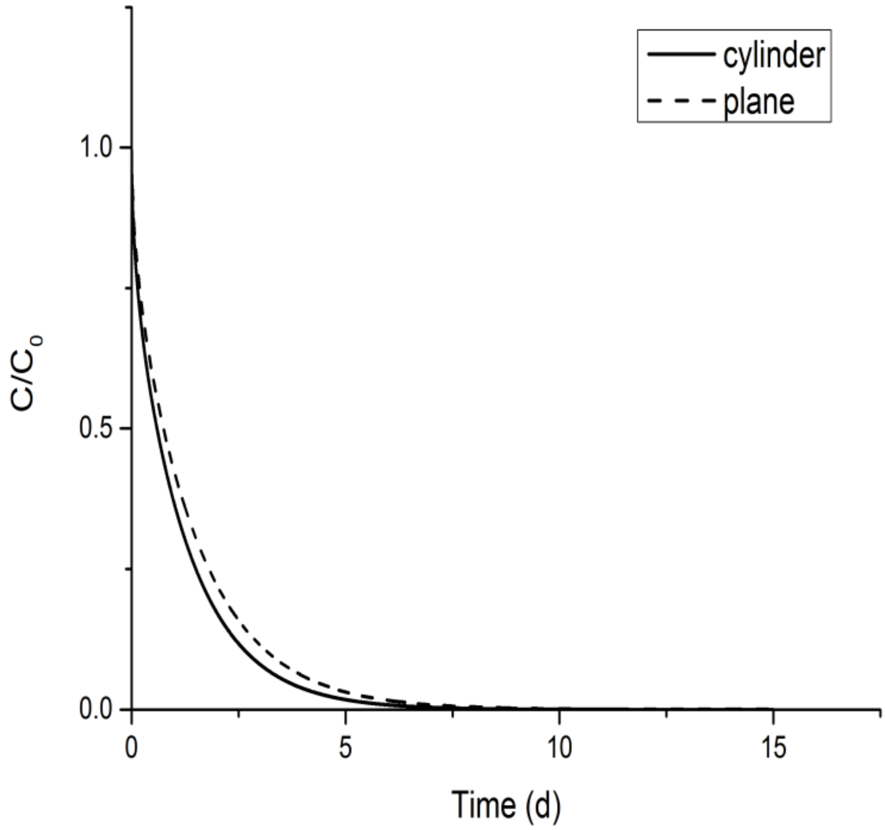


Fig. 4. The concentration of TVOC in particleboard with a thickness of 0.5 cm

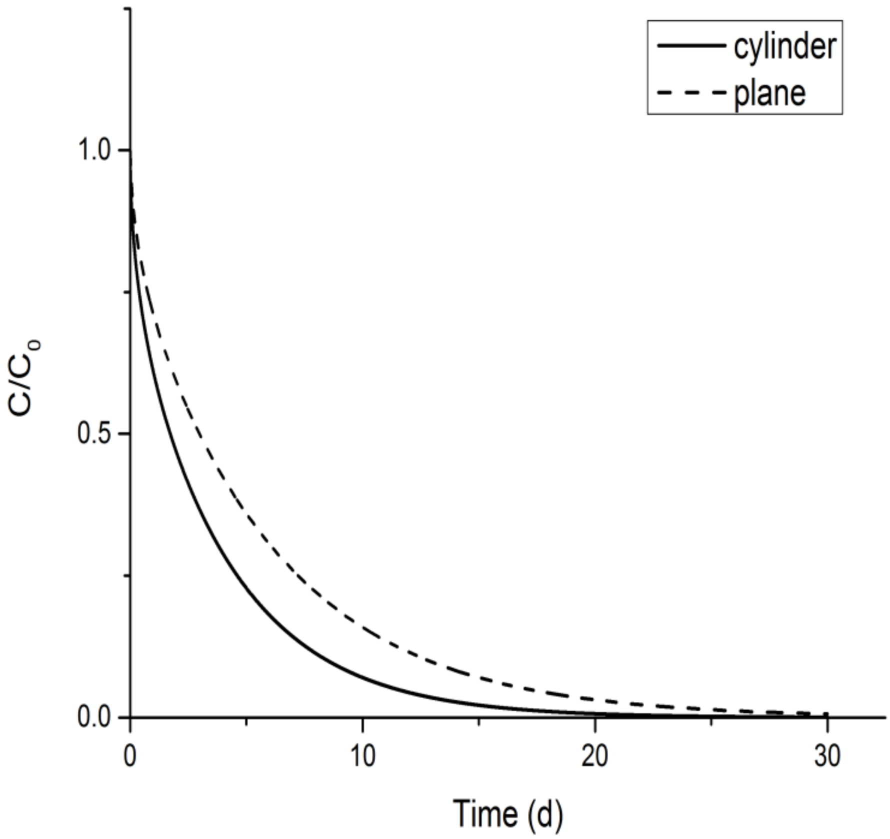


Fig. 5. The concentration of TVOC in particleboard with a thickness of 1 cm

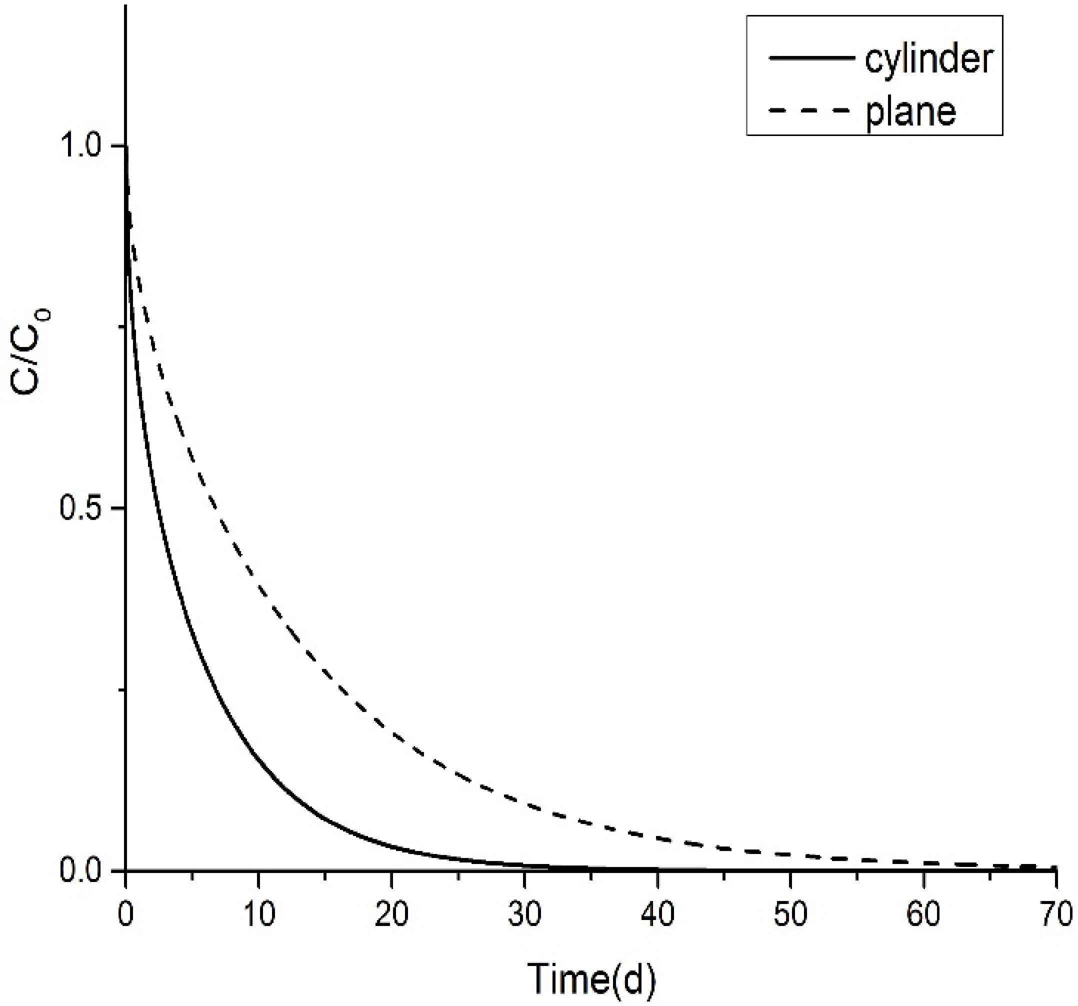
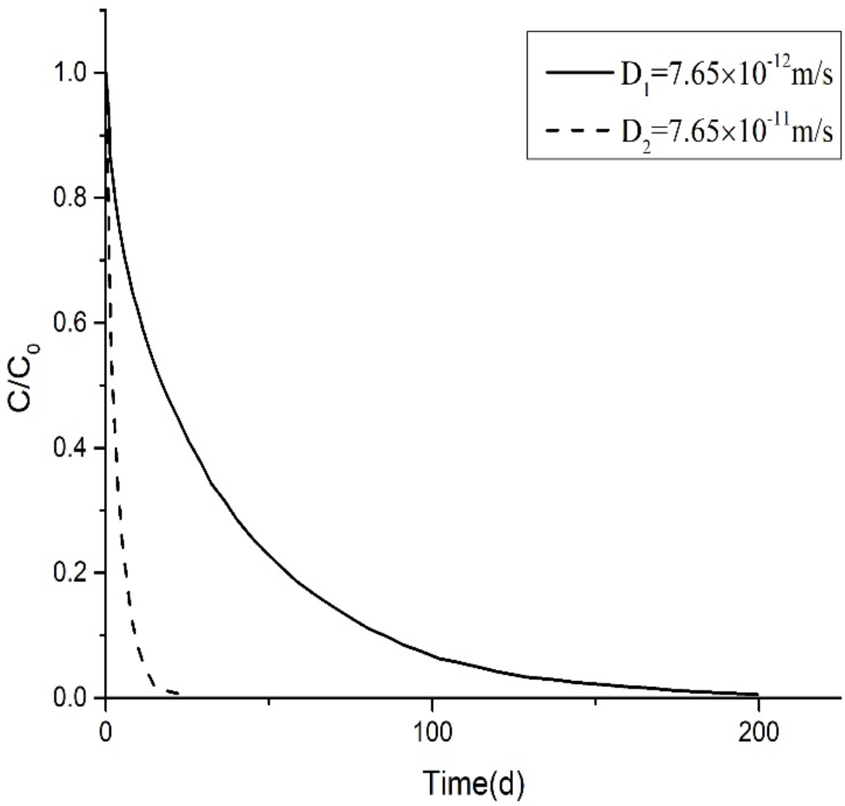


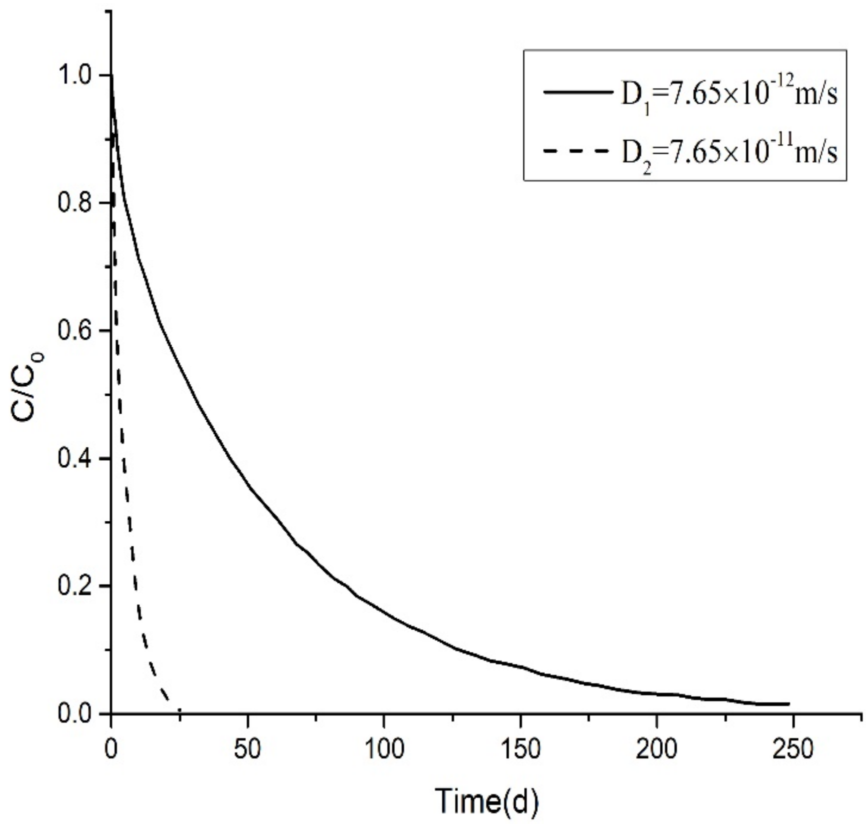
Fig. 6. The concentration of TVOC in particleboard with a thickness of 1.5 cm

The effect of diffusion coefficient

Fig. 7 shows the effect of diffusion coefficient on the emission of TVOC from two shapes of materials. The thickness of building materials is 1 cm for two shapes. The volume-averaged concentrations of TVOC in the material gradually decreases with the increase of time until it tends to the dynamic equilibrium. When the diffusion coefficient is 7.65×10^{-12} m^2/s, the non-dimensional concentration of TVOC in the planar materials is still greater than zero after 250 days, while the non-dimensional concentration of TVOC in the hollow cylindrical materials reach zero around 200 days. When the diffusion coefficient is 7.65×10^{-11} m^2/s, the non-dimensional concentration of TVOC in the planar building materials takes about 30 days to approach zero, while the non-dimensional concentration of TVOC in the hollow cylindrical materials approaches zero around 25 days. Therefore, The effect of material shape increases with the decrease in the diffusion coefficient.



(a) planar material



(b) hollow cylindrical material

Fig. 7. TVOC concentration in particleboard with different diffusion coefficients

Conclusion

This study numerically investigates the TVOC emission from planar and hollow cylindrical particleboard using CFD. The results show that emission of TVOC from hollow cylindrical material is faster than that from the planar material. With the increase of material thickness, the emissions from both the planar material and the hollow cylindrical material last for a long time. When the material thickness is relatively big, the difference in the emission from the planar material and the hollow cylindrical material tends large. Much care should be taken when simplifying the hollow cylindrical material to the planar material. The diffusion coefficient has a big effect on the emission from the planar material and the hollow cylindrical material. The effect of material shape increases with the decrease in the diffusion coefficient.

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Competing interests

The authors declare that there are no competing interests.

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Ethical considerations

“Ethical issues (Including plagiarism, Informed Consent, misconduct, data fabrication and/ or falsification, double publication and/ or submission, redundancy, etc.) have been completely observed by the authors.”

References

1. Cox SS, Zhao D, Little JC. Measuring partition and diffusion coefficients for volatile organic compounds in vinyl flooring. Atmospheric Environment. 2001 Aug 1;35(22):3823-30.

2. Katsoyiannis A, Leva P, Kotzias D. VOC and carbonyl emissions from carpets: A comparative study using four types of environmental chambers. Journal of Hazardous Materials 2008;152:669–76.

3. Da Silva CF, Stefanowski B, Maskell D, Ormondroyd GA, Ansell MP, Dengel AC, Ball RJ. Improvement of indoor air quality by MDF panels containing walnut shells. Building and Environment. 2017 Oct 1;123:427-36.

4. Horr Y A, Arif M, Kaushik A, Mazroei A, Katafygiotou M, Elsarrag E. Occupant productivity and office indoor environment quality: A review of the literature. Building and Environment 2016;105:369–89.

5. Steinemann A, Wargocki P, Rismanchi B. Ten questions concerning green buildings and indoor air quality. Building and Environment 2017;112:351–8.

6. Hu J, Li N, Yoshino H, Yanagi U, Hasegawa K, Kagi N, He Y et al. Field study on indoor health risk factors in households with schoolchildren in south-central China. Building and Environment 2017;117:260–73.

7. Deng B, Zhang B, Qiu Y. Analytical solution of VOCs emission from wet materials with variable thickness. Building and Environment 2016;104:145–51.

8. Ye W, Won D Y, Zhang X. Practical approaches to determine ventilation rate for offices while considering physical and chemical variables for building material emissions. Building and Environment 2014;82:490–501.

9. Nasreddine R, Person V, Serra C A, Schoemaecker C, Calvé S L. Portable novel micro-device for BTEX real-time monitoring: Assessment during a field campaign in a

low consumption energy junior high school classroom. Atmospheric Environment. 2016;126:211–7.

10. Chang JC, Tichenor BA, Guo Z, Krebs KA. Substrate effects on VOC emissions from a latex paint. Indoor Air. 1997 Dec;7(4):241-7.

11. Lee YK, Kim HJ. The effect of temperature on VOCs and carbonyl compounds emission from wooden flooring by thermal extractor test method. Building and Environment 2012;53:95–9.

12. Zhang JS, Nong G, Shaw CY, Wang J. Measurements of volatile organic compound (VOC) emissions from wood stains using an electronic balance. Transactions-American society of heating refrigerating and air conditioning engineers. 1999 Jul 1;105:279-88.

13. Jiang C, Li D, Zhang P, Li J, Wang J, Yu J. Formaldehyde and volatile organic compound (VOC) emissions from particleboard: Identification of odorous compounds and effects of heat treatment. Building and Environment 2017;117:118–26.

14. Cox SS, Little JC, Hodgson AT. Measuring concentrations of volatile organic compounds in vinyl flooring. Journal of the Air & Waste Management Association. 2001 Aug 1;51(8):1195-201.

15. Frihart CR, Wescott JM, Chaffee TL, Gonner KM. Formaldehyde Emissions from Urea-Formaldehyde- and no-added-formaldehyde-Bonded particleboard as Influenced by Temperature and Relative Humidity. Forest Products Journal 2012;62(7-8):551–8.

16. Afshari A, Lundgren B, Ekberg LE. Comparison of three small chamber test methods for the measurement of VOC emission rates from paint. Indoor Air 2003;13(2):156–65.

17. Brown SK. Chamber Assessment of Formaldehyde and VOC Emissions from Wood-Based Panels. Indoor Air. 1999;9(3):209–15.

18. Low JM, Zhang JS, Plett EG, Shaw CY. Effects of airflow on emissions of volatile organic compounds from. ASHRAE Transactions. 1998;104(2):1281-8.

19. Little JC, Hodgson AT, Gadgil AJ. Modeling emissions of volatile organic compounds from new carpets. Atmospheric Environment. 1994;28(2):227–34.

20. Xu Y, Zhang Y. An improved mass transfer based model for analyzing VOC emissions from building materials. Atmospheric Environment 2003;37(18):2497–505.

21. Deng B, Kim CN. An analytical model for VOCs emission from dry building materials. Atmospheric Environment 2004;38(8):1173–80.

22. Huang H, Haghighat F. Modelling of volatile organic compounds emission from dry building materials. Building and Environment 2002;37(11):1127–38.

23. Yang X, Chen Q, Zhang JS, Magee R, Zeng J, Shaw CY. Numerical simulation of VOC emissions from dry materials. Building and Environment 2001;36(10):1099–107.

24. Kumar D, Little JC. Characterizing the source/sink behavior of double-layer building materials. Atmospheric Environment 2003;37(39-40):5529–37.

25. Deng B, Tang S, Kim JT, Kim CN. Numerical modeling of volatile organic compound emissions from multi-layer dry building materials. Korean Journal of Chemical Engineering. 2010 Jul;27(4):1049-55.

26. Zhang LZ, Niu JL. Modeling VOCs emissions in a room with a single-zone multi-component multi-layer technique. Building and Environment 2004;39(5):523–31.

27. Hu HP, Zhang YP, Wang XK, Little JC. An analytical mass transfer model for predicting VOC emissions from multi-layered building materials with convective surfaces on both sides. International Journal of Heat and Mass Transfer. 2007;50(11-12):2069–77.

28. Wang X, Zhang Y. General analytical mass transfer model for VOC emissions from multi-layer dry building materials with internal chemical reactions. Chin. Sci. Bull. 2011;56(2):222–8.

29. Xu Y, Little JC. Predicting emissions of SVOCs from polymeric materials and their interaction with airborne particles. Environmental science & technology. 2006 Jan 15;40(2):456-61.

30. Wu Y, Cox SS, Xu Y, Liang Y, Won D, Liu X, Clausen PA et al. A reference method for measuring emissions of SVOCs in small chambers. Building and Environment. 2016;95:126–32.

31. Liu Z, Ye W, Little JC. Predicting emissions of volatile and semivolatile organic compounds from building materials: A review. Building and Environment 2013;64:7–25.

32. Wu, Y., Xie, M., Cox, S. S., Marr, L. C., & Little, J. C. A simple method to measure the gas-phase SVOC concentration adjacent to a material surface. Indoor Air. 2016;26:903-912.

33. Yang X, Chen Q, Zhang JS, Magee R, Zeng J, Shaw CY. Numerical simulation of VOC emission from dry materials. Building and Environment 2001;36(10):1099–107

34. Liu Z, Yan Y, Liu T, Zhao Y, Huang Q, Huang Z. How to predict emissions of volatile organic compounds from solid building materials? A critical review on mass transfer models. Journal of environmental management. 2022 Jan 15;302:114054.