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CFD analysis of SVOC mass transfer in different chambers

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ABSTRACT

Semi-volatile organic compound (SVOC) in indoor environment is an important research topic because of their wide use and persistent effect on human health. SVOC chambers have been continually improved to study the mass transfer characteristics in indoor environment. CFD method is used in the present paper to study the effect on mass transfer, especially on steady time by velocity field from the comparison of SVOC mass transfer in two different SVOC chambers (A and B). The results indicate that the variance of air flow in small range strongly affects the steady concentration and has no obvious effect on steady time. Sorption ability itself has great impact on steady time. The great reduction of steady time in Chamber B is the combined effect of sorption and velocity field. The velocity field resulted from the special structure of Chamber B leads to a stronger convective mass transfer resistance, and hence causes a weaker effective sorption. Therefore, the less steady time in Chamber B is the result of weaker effective sorption besides a less sorption area of Chamber B than Chamber A.

1. Introduction

Semi-volatile organic compounds (SVOCs) are ubiquitous in the indoor environment, and can be found from things such as vinyl flooring, wall covering, floor tiles, furniture, and electronics [1]. A man keeps exposure to indoor air for about 90% time per day [2], and exposures to SVOCs can occur via inhalation, ingestion and dermal pathways, which straightly impact on human health. Studies [2–5] suggest that exposure to semi-volatile organic compounds (SVOCs) has been associated with adverse health effects such as asthma, rhinitis, allergy and reproductive toxicity. Especially for children, SVOCs even could relate to respiratory disease and growth in developing tissue, effect on the development of male reproductive tract, prenatal mortality, and reduce growth and birth weight [6]. Phthalate, as a main kind of SVOCs, has been widely used as plasticizers to enhance the flexibility of polyvinylchloride (PVC) products [7]. These phthalates include butyl decyl phthalate (BDP), di(2-ethylhexyl) phthalate (DEHP), di(n-octyl) phthalate (DNOP), diisooctyl phthalate (DIOP) and n-Octyl n-decyl phthalate (ODP), etc. Despite of the tremendous threat to human health, phthalates are produced at a large rate of several billion tons/yr. within a decade [8]. Therefore, understanding the transport and environmental fate of phthalates in the indoor environment is significant to human health.

Experiments in chambers are the main method to characterize the fate and transport of phthalates. Destaillats et al. (2008) [9] summarized some standard chambers designed for air pollutants, such as ozone, carbonyls, volatile organic compounds (VOCs) and particles. Among these chambers, the FLEC (Field and Laboratory Emission Cell) [10–12] and CLIMPAQ (Chamber for Laboratory Investigations of Materials, Pollution, and Air Quality) [13–15] have been widely used to study the emission of VOCs. The research methods and experimental chambers on transport characteristics for SVOCs are inherited from those for VOCs. Clausen et al. [16] studied the characteristics of DEHP emission from PVC flooring and sorption on dusts in CLIMPAQ and FLEC. Xu and Little (2006) [17] developed a comprehensive mass transfer model of SVOCs in the indoor environment based on the experiments in the same two chambers. Based on the SVOC model, Clausen et al. furtherly studied the influences of humidity [18] and temperature [19] on the emission and gaseous concentration. With increasing in-depth studies of SVOCs transport, the disadvantages of the experiments in these chambers become more obvious. For example, the time to steady state for VOCs is only several hours [20], but it takes more than a hundred of hours for SVOCs [19]. SVOCs have high boiling points and low saturated vapor pressures (between 10^{-14} and 10^{-4} atm) [21]. They hence release from the source in an extremely low concentration, and tend to sorb on indoor surface and particles. Some researchers indicated that surface sorption

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could influence the time to reach steady state [22,23]. Xu et al. (2012) [23] thus developed a specially-designed chamber by maximizing the ratio of emission surface area to sorption surface area. The specially-designed chamber (Chamber A, Fig. 1(a)) effectively reduced the time to reach steady state for phthalates from 150 days in FLEC to less than 30 days. Liang and Xu (2014) [7] further improved the chamber (Chamber B, Fig. 1(b)) based on the same theory. The time to reach steady state for phthalates was sharply reduced to 5 days, which greatly saved the experimental time.

Although some achievements on research in chambers have been obtained, the properties of SVOCs strongly impede the further research. The low gaseous concentration in the chamber strongly affects the experimental accuracy. For example, the DEHP gaseous concentration in FLEC at room temperature is below 1 μg/m^3 [18], and the concentration at a temperature of 55 °C is still only 91 μg/m^3 [19]. The DEHP gaseous concentration emitted from the PVC flooring with a DEHP weight percentage of 20% at room temperature is only 2.37 μg/m^3 [7]. The long sampling time due to low gaseous concentration also has an impact on the experimental sensitivity and thus further in-depth experiments. Even in the specially-designed chamber (Chamber A in Fig. 1), a sampling duration of 24 h is still needed by a sampling pump [7]. Despite those difficulties, some problems about SVOC transport are urgently needed to study. Additionally, the further specially-designed chamber (Chamber B in Fig. 1) couldn't obtain such a tremendous reduction of time for gaseous SVOCs to reach steady state only because of its less sorption surface. The velocity field in the chamber could also play a significant role in it. Moreover, although sorption by the chamber surface is considered to have strong effect on the time to reach steady state, there is actually no detailed study ever focusing on it. At this point of time no efficient and effective experimental method exists to study the effect on the time to reach steady state by velocity field. Furthermore, the low experimental sensitivity resulted from low gaseous concentration and long sampling time couldn't allow comprehensive experiments upon the effects by surface sorption. Therefore, research conclusions by experiments are very limited. Thus CFD methods including FVM and lattice Boltzmann method (LBM) can be employed to study the mass transfer characteristics of SVOCs. Li et al. (2015) [24], Mu et al. (2015) [25] and Hussain et al. (2015) [26] adopt the technique of LBM to obtain some significant transport information, which greatly overcome the measurement difficulties in experiments. But for some macro transport problems and large-scale irregular calculation domain, FVM may still be the best approach.

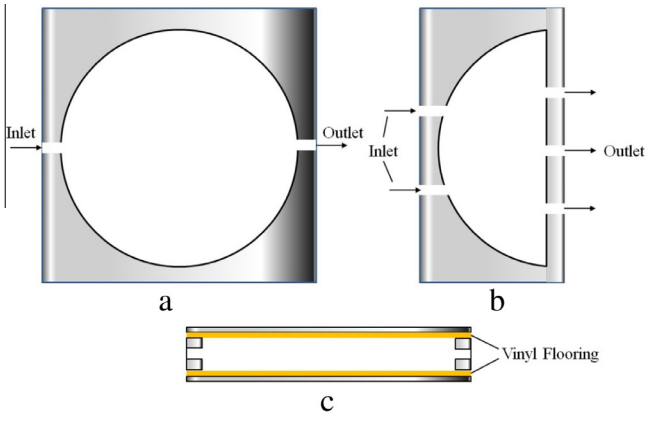

Fig. 1. Configurations of the SVOC chambers; (a) Chamber A; (b) Chamber B; (c) side view of Chamber A.

Due to experimental difficulty, there is no study to research SVOC mass transfer characteristics from the perspective of velocity field. This paper used the tool of CFD to compare the velocity field in Chamber A and Chamber B, and tried to find the intrinsic reason for sharp reduction of time to steady state from the perspective of velocity field. The simulated results were compared with reported experimental data. The effects by air flow and surface sorption were studied. Meanwhile, we also intended to reveal more mass transfer mechanism of SVOCs by comparing different transport characteristics in the two chambers.

2. Physical/mathematical models and numerical method

2.1. Physical model

The top views of Chamber A and Chamber B are shown in Figs. 1 (a) and (b), respectively. The two chambers from the side view are the same (Fig. 1(c)). The chamber is made of stainless steel, and placed between vinyl flooring (VF) sheets. The two chambers have a height of nearly 2 cm and a diameter of 20 cm (Table 1). Some special measures are taken to ensure the chamber being completely sealed. The detailed measures and design can be seen in Wu et al. [27]. Fresh air comes in through the inlet and flows out through the outlet. The two VF sheets are the only source of SVOC. The SVOC emits from the VF sheets, and is dispersed in the air. Part of them is adsorbed onto the chamber wall. The other flows out with the air through the outlet. The air flow in the cavity is laminar. The specific parameters of flow and SVOC transport are shown in Table 1.

The whole mass transport process of SVOC is shown in Fig. 2, which includes the process of emission from the floor, dispersion in the air and sorption on the wall. The diffusion within the source material could be ignored, because the emission of SVOCs from the floor is subject to "external" control [16]. Ekelund et al. [28,29] indicated that a thin film existed on the emission surface, and the SVOCs concentration in the film was kept constant [19,30]. Therefore, in the CFD model the diffusion of SVOCs in the material is not considered, and the SVOCs is assumed to be emitted from a boundary with a constant concentration. Thus the emission surface is treated as a first kind boundary condition, and SVOC enter into the simulation domain through the boundary.

2.2. Mathematical model of air flow

The air flow in the chamber can strongly impact the transport of SVOCs in the air. For incompressible flow, the conservation equations for the continuity and momentum are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0 \tag{1}$$

Table 1
Experimental conditions and model parameters.

Parameter	Chamber A	Chamber B
Temperature (°C)	22	25
Chamber volume (L), V	2	1
Air flow rate (mL/min), Q	850	1000
Air exchange rate (1/h)	25	53
Area of test pieces (m^2), A	0.252	0.13
Chamber height (cm)	2	1.8
Loading (m^2/m^3),	126	126
Concentration in equilibrium with vinyl flooring (μg/m^3), C_0	1.1	2.3
Sorption surface/air partition coefficient (m), K_s	1800	1500