Atmospheric Environment 79 (2013) 695–704

Contents lists available at ScienceDirect

Atmospheric Environment

journal homepage: www.elsevier.com/locate/atmosenv

Influence of suspended particles on indoor semi-volatile organic compounds emission

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HIGHLIGHTS

- The adsorption of suspended particles is considered for SVOCs transport in the air.
- SVOCs diffusion in particles can be described by the lumped parameter method.
- A model of SVOCs transport in the air with suspended particles is established.
- The gas-phase DEHP concentration increases rapidly in the first few seconds.
- Increasing ACH can effectively reduce the particle-phase concentration of SVOCs.

ARTICLE INFO

Article history:
Received 14 March 2013
Received in revised form
6 June 2013
Accepted 5 July 2013

Keywords:
Indoor air
Semi-volatile organic compounds
Suspended particle
Transport mechanism
Adsorption

ABSTRACT

Semi-volatile organic compounds (SVOCs) have been attracting more and more attentions to many researchers in these years. Because SVOCs have a strong tendency for adsorption to suspended particles, we take the effect of suspended particles into account to study the transport mechanism of SVOCs in the air. We establish a mathematical model to describe the transport mechanism of SVOCs, and study the transport processes of both gas- and particle-phase di-2-ethylhexyl phthalate (DEHP) in Field and Laboratory Emission Cells (FLECs). The predictions by the proposed model not only fit well with the experimental data of previous studies, but also show that the gas-phase DEHP concentration increases rapidly in the first few seconds and increases slowly during the following 200 days due to different transport mechanisms in the two periods. Meanwhile, when the particle radiuses are of the order of micron and the air changes per hour (ACH) is large enough, the characteristic time for DEHP getting gas/particle equilibrium is much longer than the residence time of a particle in the flow field, and thus there is no significant influence of suspended particles on the total concentration of DEHP in the air. Oppositely, the influence of particles on DEHP emission will be enhanced for a cycling air flow system with a small ACH, where increasing ACH will reduce the concentrations of particle-phase SVOCs. Besides, if the particle radiuses are of the order of nanometer, decreasing the particle radiuses will shorter the characteristic time for DEHP getting gas/particle equilibrium, and finally increase the particle-phase concentration of DEHP.

1. Introduction

A man keeps in contact with indoor air for about 90% time per day (Robinson and Nelson, 1995), and hence human health is straightly impacted by indoor air quality (IAQ) (Jones, 1999). The factors influencing IAQ mainly include volatile inorganic compounds, e.g. ammonia, carbon monoxide, and sulfur dioxide, volatile organic compounds (VOCs), e.g. formaldehyde, acetone, and aromatic hydrocarbon, semi-volatile organic compounds (SVOCs), e.g. di-2-ethylhexyl phthalate, pyrene, and polycyclic aromatic hydrocarbons, and inhalable particles (Brooks et al., 1991). Among the studies of these indoor pollutions, it is merely 20 years since researchers began to study on indoor SVOCs pollution (Loock et al., 1993).

According to the World Health Organization (WHO)'s classification for indoor organic compounds (WHO, 1989), SVOCs feature high boiling points and low saturated vapor pressures. They originate from many kinds of sources such as polyvinylchloride (PVC)

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http://dx.doi.org/10.1016/j.atmosenv.2013.07.010

plastic products with plasticizers and house furnishings with fire-retardants, and will cause serious harm to human health. For example, SVOCs are able to get into human blood through lung or skin and lead to several kinds of diseases, especially asthma and allergic (Bornehag and Nanberg, 2010; Jaakkola et al., 2004; Lyche et al., 2009; Kolarik et al., 2008). They will also affect the reproductive development and neurological development of human beings (Lottrup et al., 2006; Swan, 2006; Larsson et al., 2009; Testa et al., 2012).

Recent years, a considerable number of investigations on SVOCs pollution status have been brought out. Xie et al. (2005), Teil et al. (2006), Schnelle-Kreis et al. (2007), Bessagnet et al. (2010), and Wang et al. (2010) have reviewed the SVOCs pollution situation affected by various factors in different areas, such as the US, Canada, some countries in Europe, and China. Weschler (2009) reviewed the indoor pollutants since the 1950s, indicated that the pollution of phthalate esters has increased and remains high these years. On the other hand, some other researchers focused on the transport mechanism of SVOCs in the air. Xu and Little (2006) extended the model that predicts the emission rate of VOCs to predict that of SVOCs from polymeric materials, which showed reasonable agreement between the experimental data and the model predictions. Clausen et al. (2004, 2007) studied the emission of di-2-ethylhexyl phthalate (DEHP) from a PVC floor in a Field and Laboratory Emission Cell (FLEC) and a Chamber for Laboratory Investigations of Materials, Pollution, and Air Quality (CLIMPAQ), and indicated that the emission rate of DEHP was limited by gas-phase mass transport. Xu et al. (2009, 2012) did more chamber studies to elucidate the transport mechanisms of SVOCs in the air. They focused on the influence of surface adsorption on the variation of gas-phase DEHP concentration, and found that the strong partitioning of DEHP onto the stainless steel surface follows a simple linear relationship. Moreover, in order to overcome the difficulty for researchers to measure and estimate the concentrations of SVOCs promptly and accurately in experiments, Clausen et al. (2010, 2012) employed the numerical simulation to interpret the experimental results of emission of DEHP in a FLEC, and indicated that the steady-state concentrations of DEHP in the FLEC increased greatly with the increasing ambient temperature, because the adsorption to the chamber walls decreased greatly.

Besides gas-phase state, it is well-recognized now that SVOCs are quite likely to be adsorbed by particulate matters, which results in a significant effect on indoor SVOCs pollution. For the influence mechanism of suspended particles in the transport of SVOCs, Xu and Little (2006) examined the effect of SVOCs partitioning onto airborne particles, and found that airborne particles may play an important role in SVOCs transport and inhalation exposure. Weschler and Nazaroff (2008) indicated that SVOCs with low vapor pressures (or large octanol–air partition coefficients) can partition meaningfully between the gas phase and airborne particles. When the particles are smaller, their sorption to SVOC will be stronger, and the perniciousness will be more serious. Liu et al. (2012, 2013) studied the dynamic interaction between SVOCs and organic particles, and indicated that the instantaneous equilibrium assumption is not reasonable for the less volatile species such as DEHP. Benning et al. (2013) used the emission chambers designed by Xu et al. (2012) to study the influence of ultra-fine particles on the emission of DEHP, and indicated that the total (gas plus particle) DEHP concentrations increased by a factor of 3–8 when particles were introduced to the chamber at concentrations of 100–245 μg m^{-3}.

The experiments in the above studies focus mainly on the particles that are in the steady state. In other words, the SVOCs concentration has reached gas/particle equilibrium already in these studies. However, few papers focused on the influence of suspended particles on the transient emission mechanism of SVOCs in the air. In this paper, we presented a transport model of indoor SVOCs both in gas- and particle-phases, and studied SVOCs' emission in a FLEC using numerical simulations. Finally, we analyzed the influence of multiple factors, including particle number density, particle size, and air change rate, on the transport of SVOCs.

2. Transport mechanism of indoor SVOC

As discussed above, indoor airborne SVOCs exist in two phases: the gas-phase SVOCs dispersing in the air, and the particle-phase SVOCs deposited in suspended particles. Convective mass transfer occurs among the gas-phase SVOCs in the air, while particle-phase SVOCs diffuse in the suspended particles and move with them together. Meanwhile, mass transfer of SVOCs occurs between the particles and the surrounding air. In the subsequent, we will discuss the issues in the following order: the diffusion mechanism of particle-phase SVOCs, gas-phase SVOCs, the mass transfer between the particle- and the gas-phase of SVOCs, and the boundary conditions.

2.1. Diffusion mechanism of SVOC in particles

In order to study the transport mechanism of SVOCs in the air with suspended particles, it is necessary to study the diffusion mechanism of particle-phase SVOCs in particles at first. Liu et al. (2013) have studied on the mechanism of different kinds of real particles adsorbing SVOCs. As the main concern of this paper is the transport mechanism of SVOCs in the air with suspended particles, we adopt the simplest particle model for simplicity, i.e. a uniformly porous, adsorbing sphere without non-adsorbing inner core, as shown in Fig. 1.

In spherical coordinates, the conservation of a SVOC during diffusion gives

$$\frac{\partial C_p}{\partial t} = D_p\left(\frac{\partial^2 C_p}{\partial r^2} + \frac{2}{r}\frac{\partial C_p}{\partial r}\right). \tag{1}$$

The initial conditions and the boundary conditions are

$$C_p(r,t)\big|_{t=0} = 0, \tag{2}$$

$$\left.\frac{\partial C_p(r,t)}{\partial r}\right|_{r=0} = 0, \tag{3}$$

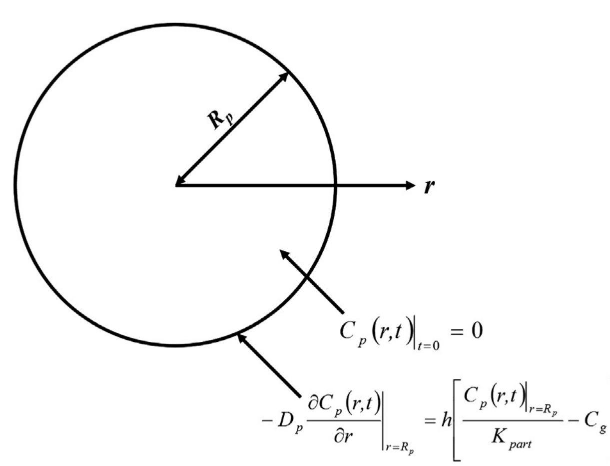

Fig. 1. The radial diffusion model in particles.