Influence of airborne particles on convective mass transfer of SVOCs on flat surfaces: Novel insight and estimation formula

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ABSTRACT

Impact of airborne particles on convective mass transfer coefficient (h_m) of semivolatile organic compounds (SVOCs) at flat surfaces has been investigated by assuming gas-particle equilibrium partition. In realistic indoor environments, however, this equilibrium partition might not be attained because the time required to reach equilibrium could be longer than residence time of airborne particles. No quantitative result of influence of particles on h_m under a non-equilibrium state has been given yet. A mass transfer model was used in this study to quantify this influence for the laminar air flow. The influence, calculated as ratio of h_m with particles present to h_m with particles absent, ε, was found to significantly depend on three dimensionless parameters: Bi_p, R, and $C_p^*(\infty)$. Bi_p represents the ratio of mass transfer rate between gas- and particle-phases SVOCs to mass transfer rate of gas-phase SVOCs transporting across the concentration boundary layer, R is the ratio of SVOC mass in particle-phase to that in gas-phase at equilibrium state, and $C_p^*(\infty)$ characterizes non-equilibrium degree of particle-phase SVOCs in the bulk air (higher non-equilibrium degree as it deviates further away from one, as one corresponds to equilibrium). At equilibrium state ($C_p^*(\infty) = 1$), the presence of particles enhances h_m ($\varepsilon > 1$) to the same extent for source surfaces and sink ones. At non-equilibrium state, ε varies linearly as $C_p^*(\infty)$ changes ($C_p^*(\infty) > 1$ for source surface, and $C_p^*(\infty) < 1$ for sink surface). The presence of particles always enhances h_m for SVOC source surfaces. In contrast, it can either enhance ($\varepsilon > 1$) or weaken ($0 < \varepsilon < 1$) h_m for sink surfaces, depending on non-equilibrium degree between gas-phase SVOCs and particles (characterized by $C_p^*(\infty)$). An empirical formula relating ε with these three parameters was obtained. Good agreement between predictions by the formula and experimental results in the literature moderately supported its reliability. Results of this study could be useful in better estimating indoor SVOC concentrations, as well as assessing and controlling human exposure to indoor SVOCs.

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1. Introduction

Human exposure to semivolatile organic compounds (SVOCs), such as phthalates, polychlorinated biphenyls, and flame retardants, has been associated with various adverse health effects, e.g., endocrine disrupting [1,2], asthma [3], and quality declining of sperms [4]. Indoor surfaces (including both source and sink surfaces) play an important role in the transport of SVOCs indoors and the subsequent human exposures [5–7]. Several studies have investigated emissions of SVOCs from indoor materials [8–12], and some others have focused on sorption of SVOCs onto sinks [13–17].

Particles can sorb a large amount of SVOCs [13] and significantly influence indoor SVOC concentrations and exposure [9,18–20]. Recently, several studies found that airborne particles may enhance mass transfer of SVOCs from/to surfaces. Weschler and Nazaroff [21] suggested that airborne particles with sorbed SVOCs in a concentration boundary layer adjacent to skin oil may accelerate mass transfer rate of SVOCs from air to skin oil. Based on mathematical model analysis, Xu and Little [9] concluded that airborne particles may decrease the SVOC gas-phase concentration in the bulk air and consequently increase the emission rate of SVOCs from source materials. Their result was confirmed by Benning et al. [22] with an experiment of DEHP (di(2-ethylhexyl) phthalate, a commonly used plasticizer indoors) emitted from vinyl flooring, which indicated that the emission rate was increased when introducing particles to their chamber with mass

Nomenclature

A	area of source surfaces	R	ratio of SVOC concentration in particle-phase to gas-phase
A_p	surface area of a single particle		
Bi_p	the ratio of mass transfer rate	Re	Reynolds number
C_g	gas-phase SVOC concentration	Sc	Schmit number
$C_{g,0}$	gas-phase SVOC concentration near the surface	U	velocity vector
$C_{g,\infty}$	concentration of gas-phase SVOC in free stream	U_∞	velocity of bulk air
C_g^*	dimensionless gas-phase SVOC concentration	V	volume of the room
C_p	SVOC concentration in a particle	V_p	volume of a single particle
$C_{p,\infty}$	particle-phase concentration of SVOC in free stream	v_t	mass transfer coefficient between gas-phase SVOCs and particles
C_p^*	dimensionless particle-phase SVOC concentration	y_0	SVOC concentration immediately adjacent to the source surface
C_{sp}	mass of particle-phase SVOC pre unit volume of air		
D_g	diffusion coefficient in the air	*Greek symbols*	
h_m	convective mass transfer coefficient	ε	ratio of $h_{m,p}$ to $h_{m,0}$
$h_{m,e}$	convective mass transfer coefficient at the source surface	ρ	density of the air
		v	kinematic viscosity coefficient
$h_{m,p}$	particle-influenced convection mass transfer coefficient		
$h_{m,0}$	convection mass transfer coefficient with particles absent	*Subscripts*	
		g	gas-phase
K	partition coefficient	p	particle
$\dot{m}$	mass transfer rate between gas- and particle-phases of SVOCs	∞	free stream
N_p	particle number concentration		
p	the pressure		
Q	ventilation rate		

concentrations of 100–245 $\mu g/m^3$. The experimental results agreed well with a mathematical model developed by Chen and Hu [23], which described SVOC transport in the air (considering dynamic interaction between gas-phase SVOCs and airborne particles). Recently, Lazarov et al. [24] also found that the presence of particles could increase the emission rate of tris (1-chloroisopropyl) phosphate (TCIPP, frequently used as flame retardant and plasticizer) by a factor of 3 based on experiments conducted in Field and Laboratory Emission Test Cell (FLEC).

Liu et al. [25] developed a steady-state mass transfer model to investigate role of particles in mass transfer of SVOCs from/to surfaces, focusing on the concentration boundary layer of gas-phase SVOCs near flat surfaces. Their analysis suggested that the concentration boundary layer thickness of gas-phase SVOCs would be reduced (i.e., enhancing the convective mass transfer coefficient (h_m) of SVOCs between bulk air and surface) due to the presence of particles [25]. Liu et al. [25] also suggested that the enhancement of mass transfer by particles was proportional to the non-equilibrium degree between gas-phase SVOCs and particles in the bulk air; however, no quantitative results were given. In realistic indoor environments, the residence time of airborne particles tends to be on the order of one hour [13,26]. For SVOCs with large particle/gas partition coefficient (K), such as DEHP with K of $10^{12.5}$ [13], the timescale required for reaching equilibrium partition between airborne particle and gas-phase SVOCs (about 10–100 h) is longer than the residence time (e.g., one hour) [13]. This means that a non-equilibrium gas-particle partition of SVOCs is quite possible. In addition, relationships between the enhancement of particle-mediated SVOC mass transfer and its influencing factors (e.g., particles size, K, air speed of the bulk air, particle concentrations, and diffusion coefficient of SVOCs in the air) was presented in the form of figures, which may be inconvenient for application.

Objectives of this study are therefore to reveal the influence of airborne particles on convective mass transfer coefficient of SVOCs from/to flat surfaces under non-equilibrium states, and to quantify this phenomenon with an empirical formula for the convenience of

application. Measured results of Benning et al. [22] are employed to evaluate the presented model and the empirical formula.

2. Mechanism and methods

2.1. Mechanism description

Similar phenomena in the heat transfer field have been analyzed by Guo et al. [27] and Hu and Zhang [28]. Due to the analog between heat transfer and mass transfer, their conclusions are considered to be applicable to mass transfer [29]. That is, considering the one-dimensional mass transfer by diffusion between two flat plates (with different concentrations) at steady state, Fig. 1(a) shows the concentration distribution between two plates without source, and Fig. 1(b) shows the case with a uniform positive source ($\dot{S} > 0$, where $\dot{S}$ is the source strength) between these two plates [27]. It can be seen that the concentration gradient rises at the boundary with lower concentration, i.e., mass diffusion rate of the lower concentration plate increases due to the existing of positive source. Analogously, a sink ($\dot{S} < 0$) may increase the mass diffusion rate of the plate with higher concentration. Furthermore, by studying the analog between convection and conduction, Guo et al. [30] found that a positive heat source inside the thermal boundary layer may increase the convective heat transfer coefficient (i.e., heat flux) for the lower temperature plate (lower compared to the temperature outside the boundary layer). Similarly, a source of mass may increase the convective mass transfer coefficient of the lower concentration plate (a sink has the same impact on the higher concentration plate).

The above conclusions are considered to be applicable to the case of this study. For SVOC emission from a source surface, gas-phase SVOC concentration immediately adjacent to the source ($C_{g,0}$) is higher than gas-phase SVOC concentration in the bulk air ($C_{g,\infty}$). Thus, if a particle with sorbed SVOCs in the bulk air moves into boundary layer above the source surface, this particle will