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Distributions of the particle/gas and dust/gas partition coefficients for seventy-two semi-volatile organic compounds in indoor environment

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HIGHLIGHTS

- 38 empirical equations to calculate K_p and K_d from p_L^0 and K_{oa} were summarized.
- A reference distribution of $\log_{10} K_p$ for 72 SVOCs was determined.
- The $\log_{10} K_p$ values were normally distributed for 27 SVOCs.
- The distribution reduces the bias in choosing a specific equation to calculate K_p.
- The ratio between K_p and K_d was determined using linear regression.

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ABSTRACT

Particle/gas and dust/gas partition coefficients (K_p and K_d) are two key parameters that address the partitioning of semi-volatile organic compounds (SVOCs) between gas-phase, airborne particles, and settled dust in indoor environment. A number of empirical equations to calculate the values of K_p and K_d have been reported in the literature. Therefore, the difficulty lies in the selection of a specific empirical equation in a given situation. In this study, we retrieved from the literature 38 empirical equations for calculating K_p and K_d values from the SVOC saturation vapor pressure and octanol/air partition coefficient. These values were calculated for 72 SVOCs: 9 phthalates, 9 polybrominated diphenyl ethers (PBDEs), 11 polychlorinated biphenyls (PCBs), 22 biocides, 14 polycyclic aromatic hydrocarbons (PAHs), 3 alkylphenols, 2 synthetic musks, tributylphosphate, and bisphenol A. The mean and median values of $\log_{10} K_p$ or $\log_{10} K_d$ for most SVOCs were of the same order of magnitude. The distribution of $\log_{10} K_p$ values was fitted to either a normal distribution (for 27 SVOCs) or a log-normal distribution (for 45 SVOCs). This work provides a reference distribution of the $\log_{10} K_p$ for 72 SVOCs, and its use may reduce the bias associated with the selection of a specific value or equation.

1. Introduction

The partitioning equilibrium of semi-volatile organic compounds (SVOCs) between gas-phase and airborne particles, and between gas-phase and settled dust in indoor environments can be described by the particle/gas partition coefficient (K_p) and the dust/gas partition coefficient (K_d), respectively (Weschler et al., 2008). At steady state, if K_p or K_d is known, unknown SVOC concentrations in the gas-phase can be calculated based on their measured concentrations in airborne particles or settled dust, respectively (Weschler and Nazaroff, 2010).

The K_p and K_d values can be obtained by measuring SVOC concentrations of gas-phase, airborne particles, and settled dust under the assumption of a partitioning equilibrium of SVOCs within these three phases. For example, Benning et al. (2013) used vinyl flooring

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placed inside a stainless steel environmental chamber as a di-(2-ethylhexyl)-phthalate (DEHP) source. They measured the DEHP concentrations in the gas-phase and airborne particles and calculated the particle/gas partition coefficient. The K_p and K_d values over a wide range of SVOCs are more frequently calculated using empirical equations that include the SVOC saturation vapor pressure (p_L^0) or the octanol/air partition coefficient (K_{oa}).

Though a large amount of work is available, two practical problems concerning the determination of K_p and K_d for SVOCs remain unsolved. First, a number of equations exist for calculating K_p and K_d values. Theoretical relationships between K_p and p_L^0 and between K_p and K_{oa} were determined by Pankow (1994) and Finizio et al. (1997), respectively. However, some physical parameters in the theoretical equations, e.g., the activity coefficient of the absorbing SVOCs in airborne particles and the fraction of the airborne particles that is organic matter, have not been fully studied for most SVOCs and their values remain assumed in these calculations (Harner, 1998). Empirical equations, which are determined based on the regression of experimental data for various compounds in a number of studies, differ in their regression constants. Finizio et al. (1997) critically reviewed 12 empirical equations that include K_p and p_L^0 and proposed equations that include K_{oa} as a sufficient descriptor to predict K_p for a number of SVOCs. Following their research study, more equations that include K_{oa} were proposed by Harner (1998), Shoeib et al. (2005), and Weschler and Nazaroff (2010). Salthammer and Schripp (2015) performed a quantitative error analysis of the Junge-Pankow equation based on parameter uncertainties, but the error in other equations remains unverified. As a result, users may encounter difficulties in the selection of an equation for the prediction of K_p, K_d and the unknown concentration of SVOCs in a given phase. Second, the relationship between K_p and K_d has not been clearly addressed. Consequently, the accuracy of the gas-phase SVOC concentrations calculated using K_p or K_d remains unverified.

To solve the problems, this work aims to provide reference distributions of $\log_{10} K_p$ and $\log_{10} K_d$ for a number of SVOCs with

Table 1

Empirical equations to calculate $\log_{10} K_p$ ($m^3\ \mu g^{-1}$) and $\log_{10} K_d$ ($m^3\ g^{-1}$) at 25 °C.

Empirical equation	Studied compounds	Reference
$\log_{10}K_p = -0.860 \log_{10}p_L^0 - 4.67$	PAHs	Naumova et al., 2003
$\log_{10}K_p = -\log_{10}p_L^0 - 5.47$	PAHs	Cotham and Bidleman, 1995; Finizio et al., 1997
$\log_{10}K_p = -0.694 \log_{10}p_L^0 - 4.61$	PAHs	Cotham and Bidleman, 1995; Finizio et al., 1997
$\log_{10}K_p = -0.81 \log_{10}p_L^0 - 5.31$	PAHs	Ngabe and Bidleman, 1992; Finizio et al., 1997
$\log_{10}K_p = -1.04 \log_{10}p_L^0 - 5.95$	PAHs	Yamasaki et al., 1982; Finizio et al., 1997
$\log_{10}K_p = -0.76 \log_{10}p_L^0 - 5.10$	PAHs	Foreman and Bidleman, 1990; Finizio et al., 1997
$\log_{10}K_p = -0.88 \log_{10}p_L^0 - 5.38$	PAHs	Ligocki and Pankow, 1989; Finizio et al., 1997
$\log_{10}K_p = -0.61 \log_{10}p_L^0 - 4.26$	PAHs	Baker and Eisenreich, 1990; Finizio et al., 1997
$\log_{10}K_p = -0.726 \log_{10}p_L^0 - 5.18$	PCBs	Cotham and Bidleman, 1995; Finizio et al., 1997
$\log_{10}K_p = -0.95 \log_{10}p_L^0 - 5.86$	PCBs	Foreman and Bidleman, 1990; Finizio et al., 1997
$\log_{10}K_p = -0.61 \log_{10}p_L^0 - 4.74$	PCBs and organochlorine pesticides	Kaupp and Umlauf, 1992; Finizio et al., 1997
$\log_{10}K_p = -0.69 \log_{10}p_L^0 - 5.06$	PCBs and organochlorine pesticides	Hoff et al., 1996; Finizio et al., 1997
$\log_{10}K_p = -0.92 \log_{10}p_L^0 - 5.63$	Organochlorine pesticides	Foreman and Bidleman, 1990; Finizio et al., 1997
$\log_{10}K_p = -0.8698 \log_{10}p_L^0 - 4.7707$	PAHs and polychlorinated naphthalenes (PCNs)	Kaupp and McLachlan, 1999
$\log_{10}K_p = -0.6027 \log_{10}p_L^0 - 5.1661$	PCBs and organochlorine pesticides	Kaupp and McLachlan, 1999
$\log_{10}K_p = -0.715 \log_{10}p_L^0 - 5.141$	PCBs	Harner, 1998
$\log_{10}K_p = -0.745 \log_{10}p_L^0 - 4.666$	PAHs	Harner, 1998
$\log_{10}K_p = -0.65 \log_{10}p_L^0 - 4.04$	PAHs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.75 \log_{10}p_L^0 - 4.35$	PAHs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.86 \log_{10}p_L^0 - 5.66$	PAHs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.76 \log_{10}p_L^0 - 4.57$	PAHs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.51 \log_{10}p_L^0 - 4.72$	PCBs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.60 \log_{10}p_L^0 - 4.93$	PCBs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.58 \log_{10}p_L^0 - 4.56$	PCBs	He and Balasubramanian, 2009
$\log_{10}K_p = -0.58 \log_{10}p_L^0 - 4.72$	PCBs	He and Balasubramanian, 2009
$\log_{10} K_p = \log_{10} K_{oa} + \log_{10}(1.88 \times 10^{-12})$	PAHs	Finizio et al., 1997; Weschler et al., 2008
$\log_{10} K_p = \log_{10} K_{oa} + \log_{10}(1.5 \times 10^{-12})$	PCBs and organochlorine pesticides	Finizio et al., 1997
$\log_{10} K_p = 0.79 \log_{10} K_{oa} - 10.01$	PAHs	Finizio et al., 1997
$\log_{10} K_p = 0.55 \log_{10} K_{oa} - 8.23$	PCBs and organochlorine pesticides	Finizio et al., 1997
$\log_{10}K_p = \log_{10}K_{oa} + \log_{10}\left(\frac{f_{om\_p}}{\rho_p}\right)$ [a]	SVOCs	Weschler and Nazaroff, 2010
$\log_{10} K_p = 0.6368 \log_{10} K_{oa} - 8.9111$	PCBs, organochlorine pesticides, PAHs, and PCNs	Kaupp and McLachlan, 1999
$\log_{10} K_p = 0.654 \log_{10} K_{oa} - 9.183$	PCBs	Harner, 1998
$\log_{10} K_p = 0.735 \log_{10} K_{oa} - 9.947$	PCNs	Harner, 1998
$\log_{10} K_p = 0.829 \log_{10} K_{oa} - 10.263$	PAHs	Harner, 1998
$\log_{10}K_p = \log_{10}K_{oa} + \log_{10}f_{om\_p} - 11.91$	SVOCs	Harner, 1998;
$\log_{10}K_d = \log_{10}K_{oa} + \log_{10}\left(\frac{0.411 f_{om\_d}}{\rho_d}\right)$ [b]	Perfluorinated alkyl sulfonamides	Shoeib et al., 2005; Weschler et al., 2008
$\log_{10}K_d = \log_{10}K_{oa} + \log_{10}\left(\frac{f_{om\_d}}{\rho_d}\right)$ [c]	SVOCs	Weschler and Nazaroff, 2010
$\log_{10} K_d = 0.86 \log_{10} K_{oa} - 6.09$	SVOCs	Weschler and Nazaroff, 2010

[a] $f_{om\_p} = 0.4$, $\rho_p = 1 \times 10^{12}\ \mu g\ m^{-3}$ (Weschler and Nazaroff, 2010).

[b] $f_{om\_d} = 0.2$ (Weschler and Nazaroff, 2010), $\rho_d = 1 \times 10^6\ g\ m^{-3}$ (Weschler et al., 2008).

[c] $f_{om\_d} = 0.2$, $\rho_d = 2 \times 10^6\ g\ m^{-3}$ (Weschler and Nazaroff, 2010).