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# Contaminant uptake by polymeric passive samplers: A modeling study with experimental validation

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## ABSTRACT

Accurate determination of contaminant partitioning in polymeric passive samplers (PPSs) is of great interest, especially for planning monitoring programs in environmental investigations. In this study, a predictive partition coefficient model is developed which only requires the chemical structures of polymer in PPSs and contaminant as input. As such, a kinetic model is developed to account for time evolution of the contaminant uptake. To analyze the performance of the developed model, experimental data were collected from literature to validate against the model. The accumulative absolute relative deviation (AARD (%)) was used in order to evaluate the goodness of predictions. Comparing the measured and calculated partition coefficients indicated an overall prediction error of 5.17%. The developed model can provide valuable information regarding polymers selection for PPSs fabrication and the time evolution of uptake process.

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## 1. Introduction

In fabrication of polymeric passive samplers (PPSs), low density polyethylene (LDPE) has been one of the most widely used polymers (Thompson et al., 2015). PPSs are mainly used to measure the concentration of hydrophobic organic compounds in water and wastewater which is then used for analyzing health risk level of water streams (Thompson et al., 2015; Adams et al., 2007; Endo et al., 2011; Lohmann and Muir, 2009; Asgarpour Khansary et al., 2017). Based on such analysis, it can be concluded that which water treatment technology should be used (Xu et al., 2016; Zanacic et al., 2016; Mahmoud et al., 2016), and practically is suitable. Development of a mathematical model to predict the performance of PPSs (Asgarpour Khansary et al., 2017) is

of much interest to reduce the costs associated with experimental analysis (Tosun, 2007; Khansary et al., 2014). Availability of an efficient mathematical models is valuable as site-related measurement faults and necessities may occur (Bergmair et al., 2014, 2015; Bar, 2004; Wahlgren, 2001; Milani et al., 2014), and these models can be used to correlate obtained data. Also, the effect of various operating parameters and design scenarios can be theoretically analyzed is another advantage of model development for PPSs (Asgarpour Khansary et al., 2017).

Experimentally measured data on polymer–water partition coefficients for various PPSs are reported in literature (Thompson et al., 2015; Adams et al., 2007; Endo et al., 2011; Lohmann and Muir, 2009), however theoretical models have been rarely noted and considered (Asgarpour

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Khansary et al., 2017). Thus, in this work attempts were made to establish a theoretical model of polymer–water partition coefficients and time evolution of contaminants uptake by PPSs. Some available experimental data reported in literature were collected and used for evaluation of the model performance. The accumulative absolute relative deviation (AARD (%)) was used to demonstrate the goodness of model predictions.

## 2. Contaminant uptake model

Contaminant uptake by polymeric passive samplers takes place in two steps; (i) sorption of species at the interface of sampler/sampling phases, and (ii) diffusion of species through the passive sampler. For the first step, partition coefficient ( $K$ ) of contaminant between the sampling phase and polymeric sampler correlates the concentration of contaminant in the sampling phase ( $c_1^I$ ) to the concentration of contaminant in polymeric sampler ( $c_1^{II}$ ) adjacent to the interface of sampling phase and polymeric sampler as defined in Eq. (1).

$$K = \frac{c_1^{II}}{c_1^I} \quad (1)$$

In a recent work (Asgarpour Khansary et al., 2017), a modeling approach for prediction of partition coefficients of PPSs was developed following the fundamental chemical thermodynamic equations governing the concerned local equilibrium using a Flory–Huggins model (Lindvig et al., 2002) based on the Hansen solubility parameters. The model of Asgarpour Khansary et al. (2017) is given in Eq. (2):

$$\begin{aligned} (c_1^I)^3 - 2 \frac{[\chi_{12}^I - \chi_{12}^{II}K]}{[\chi_{12}^I - \chi_{12}^{II}K^2]} \frac{\rho_1}{Mw_1} (c_1^I)^2 + \frac{[\chi_{12}^I - \chi_{12}^{II} + \ln \frac{1}{K}]}{[\chi_{12}^I - \chi_{12}^{II}K^2]} \\ \left[ \chi_{12}^I - \chi_{12}^{II}K^2 \right] \left( \frac{\rho_1}{Mw_1} \right)^2 c_1^I + \frac{1-K}{[\chi_{12}^I - \chi_{12}^{II}K^2]K} \left( \frac{\rho_1}{Mw_1} \right)^2 = 0 \end{aligned} \quad (2)$$

where superscripts  $I$  and  $II$  denotes the sampling phase (water, air, etc.) and the polymeric phases, respectively.  $\chi_{12}$  is the Flory–Huggins interaction parameter between compound 1 and compound 2 (in phase  $I$ : sampling phase (air, water, etc.), in phase  $II$ : polymer).  $K$  refers to the partition coefficient defined as  $K = c_1^{II}/c_1^I$  (Khansary et al., 2017a).  $Mw$  and  $\rho$  denote the molecular weight and density, respectively.

The Flory–Huggins interaction parameter used in Eq. (2), between compound 1 and compound 2 ( $\chi_{12}$ ), is given by Eq. (3) (Lindvig et al., 2002):

$$\chi_{12} = 0.6 \frac{V_1}{RT} \left[ (\delta_{d,1} - \delta_{d,2})^2 + 0.25(\delta_{p,1} - \delta_{p,2})^2 + 0.25(\delta_{h,1} - \delta_{h,2})^2 \right] \quad (3)$$

where  $V_1$ ,  $R$ , and  $T$  refer to the molar volume, universal gas constant, and temperature, respectively.  $\delta_d$  denotes dispersion contribution of Hansen solubility parameter,  $\delta_p$  polar contribution of Hansen solubility parameter, and  $\delta_h$  hydrogen-bonding contribution of Hansen solubility parameter (Lindvig et al., 2002; Khansary et al., 2017a).

In Eq. (3),  $\chi_{12}$  is the composition-independent interaction parameter in Flory–Huggins model, however it has been demonstrated (Farajnezhad et al., 2016a; Asgarpour Khansary and Aroon, 2015; Khansary and Aroon, 2015; Mejía and Segura, 2015) that a composition-dependent interaction parameter increases the predictive capabilities of Flory–Huggins model. In Khansary (2016), a model for Flory–Huggins interaction parameter was introduced by combination of regular solution model of Flory and Huggins as well as regular solution

model of Ruzette and Mayes (2001) as given in Eq. (4).

$$\begin{aligned} \chi_{12} = (\tilde{\rho}_1 - 1) \frac{\sqrt{v_1 v_2}}{N_1 v_1} \frac{\phi_1}{\phi_2} \ln \phi_1 + (\tilde{\rho}_2 - 1) \frac{\sqrt{v_1 v_2}}{N_2 v_2} \frac{\phi_2}{\phi_1} \ln \phi_2 \\ + \tilde{\rho}_1 \tilde{\rho}_2 \sqrt{v_1 v_2} (\delta_{1,0} - \delta_{2,0})^2 + (\tilde{\rho}_1 - \tilde{\rho}_2) (\delta_1^2 - \delta_2^2) \sqrt{v_1 v_2} \end{aligned} \quad (4)$$

where  $\tilde{\rho}_i$  is the reduced density which can be obtained from the modified Sanchez and Lacombe's lattice-fluid (LF) equation of state (Boudouris et al., 1997) in which the characteristic pressure and temperature are calculated using group contribution method developed by Boudouris et al. (1997).  $\delta_{i,0}$  is the hard-core solubility parameter at 0K obtained from the Hoftzyer and van Krevelen group contribution method (van Krevelen and Nijenhuis, 2008). The hard-core solubility parameter at temperature of system ( $\delta_i$ ) can be simply evaluated using  $\delta_i^2 = \delta_{i,0}^2 (\rho_i/\rho_i^0)$  where  $\rho_{i,0}$  is calculated using modified SL-EOS at STP condition.  $v_i$  is the hard-core volume;  $v_i^* = kT_i^*/P_i^*$ ,  $N_i = r_i v_i^*/\tilde{\rho}_i$  and  $r_i = Mw_i P_i^*/kT_i^* \rho_i^*$  (Lacombe and Sanchez, 1976; Sanchez and Stone, 2000; Sanchez and Lacombe, 1978).  $\phi$  is volume fraction that can be related to the concentration using  $c_i = \rho_i \phi_i / Mw_i$ .

The current modification of the model of Asgarpour Khansary et al. (2017) provides a predictive approach for calculation of both partition coefficients and compounds concentrations in each phase consistent with the nature of Flory–Huggins interaction parameter ( $\chi_{12}$ ). The employed model for composition-dependent interaction parameter implicitly incorporates regular solution model of Ruzette and Mayes (2001) into regular solution model of Flory and Huggins (Khansary, 2016), and this enhances its predictive capabilities. The versatility and reliability of regular solution model of Ruzette and Mayes (2001) for description of phase behavior of various solutions have been demonstrated in literature (Farajnezhad et al., 2016a,b; Keshavarz et al., 2015; Madaeni and Bakhtiari, 2012; Ghasemi and Mohammadi, 2013).

The steps of calculation for application of modified partition coefficient model are described below:

1. Drawing the desired components molecular structure and identifying each group/class using group contribution method of Boudouris et al. (1997),
2. Calculating lattice fluid scaling parameters ( $P^*$ ,  $T^*$  and  $\rho^*$ ) using data of step #1
3. Calculating reduced properties ( $\tilde{P}$  and  $\tilde{T}$ ) using the calculated scaling parameters from step #2 and the operating conditions of the considered system,
4. Calculation of the reduced density ( $\tilde{\rho}$ ) by iterative solution of SL-EOS using data of step #3 and initial guess of  $\tilde{\rho} = 1$ ,
5. Calculating hard-core solubility parameter at reference temperature of 298 K ( $\delta_i^2(298)$ ) using the Hoftzyer and van Krevelen group contribution method (van Krevelen and Nijenhuis, 2008),
6. Calculating hard-core solubility parameter at system temperature prior which hard-core density should be determined at system temperature as  $\rho = \tilde{\rho} \rho^*$  where  $\tilde{\rho}$  is obtained in step # 4,
7. Calculating  $N_i v_i$  model using  $N_i v_i = Mw/\rho^*$  equality, where  $Mw$  is the molecular weight of component
8. Calculating the composition-dependent Flory–Huggins interaction parameter using Eq. (4) for each phase,
9. For each partition coefficient ( $K$ ) value,

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