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New insight into advection of organic contaminate plume at drain outlet areas

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ABSTRACT

To provide insight to optimize organic contaminants treatment at the drain outlet areas due to the discharge from the industrial plants, the fate and transport of variety kinds of organic contaminants were investigated. By taking the chemical properties (molecular weight (MW), Henry's law constant (H), vapor pressure (P_v), organic carbon normalized soil-water partition coefficient for organic compounds (K_{oc}), water solubility (S), air diffusivity (Da), and water diffusivity (D_w)) of 56 kinds of organic chemical into account, we studied the general transport equation (GTE) regarding the mass balance for the steady-state analysis of the accumulation of a chemical over time by the plume advection. We found that K_{oc} has significant relationship with S and MW of the chemicals. Furthermore, higher organic carbon-water partitioning coefficient of the chemical will make it easier to stay at the drain outlet area, which gives us hints for next research of nanoscale particles for in situ remediation.

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1. Introduction

As a result of industrial practices, organic contaminants have been detected in many drain outlet areas, resulting in contaminant in crop growth, water ecological environment, clean water resource and human health, which is lack of enough concern in some developing countries (Ávila et al., 2015; Honkonen and Rantalainen, 2012; Huang et al., 2015). The need to understand the fate and transport of the organic contaminants has led to numerous studies that used various techniques including dye- and chemical tracer studies (Barns et al., 2015; Subedi et al., 2015), and simple to more complex digital or numerical transport models (Georgi et al., 2015; Simon et al., 2013). However, all of them still did not solve the movement of particular organic contaminant problems with the determination of what happens to them (e.g. when does it end up? What does it transform to? How long does it persist? etc.) by the processes of definition, model, monitor and quantifying.

Obviously, the non-uniform/non-steady-state has more problems of interest. Most of the fate and transport phenomon of the contaminants in natural or man-made systems are non-uniform and non-steady-state (Ramšak et al., 2013). However, it is difficult to define them and make models to quantify due to their un-directional concentration distribution. Moreover, the real and complex system includes solids and voids and there are lack of detailed data on its configuration within the void space (Yao et al., 2013). Thus, under some conditions, researchers just make it simple and assume it steady-state to do qualitative analysis. Luckily, researchers still could validate the model at a point within the void space by both recognizing the porous medium domain as a whole visualized as a continuum, and each of the phases and components as a continuum (Chabauty et al., 2015; Cheng and Saiers, 2015; Essaid et al., 2015). Sincerely, what more important is to win the public's concern like (Robles-Morua et al., 2012) did before. They showed that the regions in the river are in noncompliance with fresh water pathogen norms. It was shown that these risks are highly sensitive to spatiotemporal variability in river discharges and uncertainty in pathogen removal rates. Thus, the local government and people could be conscious of this series problem.

In this study, we derived the general transport equation (GTE) with the mass balance equation for the 56 kinds of organic chemicals. After solving the problem about GTE, we could get the accumulation of a substance over time within the defined control volume with the independent variables of the flux that we should assume. Specific information about chemical parameters that is
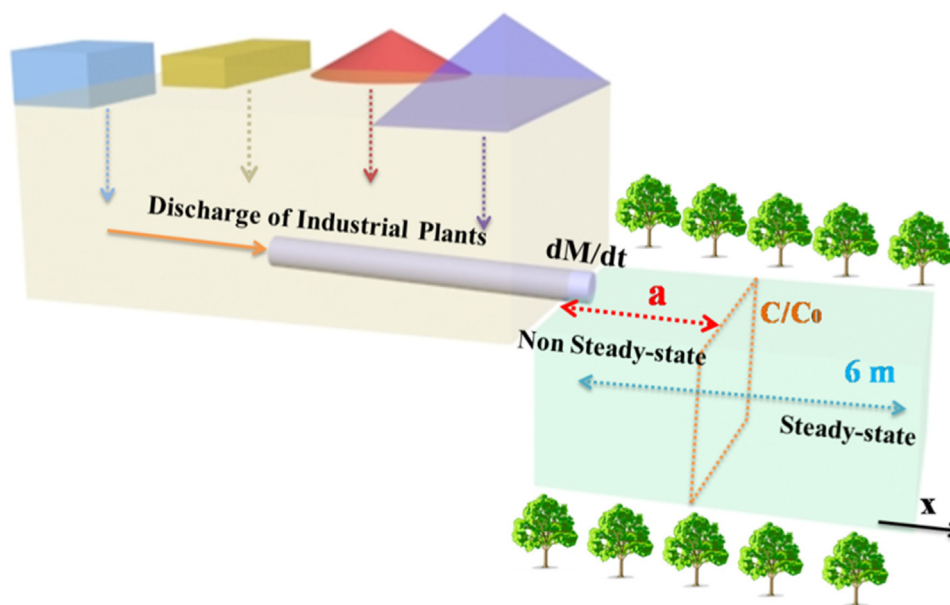
Fig. 1. Scheme of the advection model for organic chemicals at the drain outlet areas.

needed includes molecular weight (MW), Henry's law constant (H), vapor pressure (P_v), organic carbon normalized soil-water partition coefficient for organic compounds (K_{oc}), water solubility (S), air diffusivity (D_a), and water diffusivity (D_w).

2. Methodology

In order to investigate the consistency between the tabulated values in Table S1, we firstly calculated the estimated Henry's law constant H(cal) using the following equation (Lesser et al., 2008; Luo 2009):

$$H(cal) = \frac{P_v M}{RTS} \tag{1}$$

where R is the gas constant of 0.082 L-vapor atm mol^{-1} K^{-1}, T is the absolute temperature (K), P_v is the vapor pressure (atm), S is the solubility (g/L-water) and M is the molecular weight of the chemical (g/mol).

Furthermore, K_{oc} has been correlated with the aqueous solubility and the solubility gives a good first approximation of adsorption when $\log K_{oc}$ is plotted against $\log S$ for a group of organic compounds as the following equation (Shea, 1989):

$$\log k_{oc} = 3.94 - 0.50 \log S \tag{2}$$

The expressions for fraction of total mass in dissolved phase, fraction of total mass in sorbed phase, and fraction of total mass in vapor phase are shown as follows and the derivative details are included in SI:

$$fraction - dissolved = \frac{\phi_m C_m V}{\rho C_T V} = \frac{\phi_m}{H\phi_v + \phi_m + \rho K_s} \tag{3}$$

$$fraction - sorbed = \frac{\rho C_s V}{\rho C_T V} = \frac{\rho K_s}{H\phi_v + \phi_m + \rho K_s} \tag{4}$$

$$fraction - vapor = \frac{\phi_v C_v V}{\rho C_T V} = \frac{H\phi_v}{H\phi_v + \phi_m + \rho K_s} \tag{5}$$

where, in our study, C_m, C_s, C_v, and C_T are dissolved concentration (g/L^3-water), sorbed concentration (g/L^3-soil), vapor concentration (g/L^3-vapor), and total concentration (g/L^3), respectively, soil bulk density ρ=1.5 kg-soil/cm^3-soil, Φ_v = 0.2 L-vapor/cm^3-total voids,

Φ_m = 0.2 cm^3-water/cm^3-total voids, K_s = f_{oc}*K_{oc} with fraction of organic carbon f_{oc} = 0.01 g-OC/g-soil.

Using the advection model schematically illustrated in Fig. 1, the following mass balance equation could be obtained to derive the transient concentration curve (Cavanagh et al., 2014; Lundegard and Johnson, 2004):

$$\frac{dM}{dt} = C_0 q_m A - C_{600} q_m A + Re \tag{6}$$

where M is the mass of the chemical (g), t is the time (day), C_0 is the source concentration (g/L^3), q_m is the specific discharge (L^3/day/m^2), C_{600} is the concentration at 600 cm (g/L^3), A is the cross area (m^2), and Re is the reaction term (g/day).

With the assumption of steady-state and no reaction, we can obtain the following equations:

$$\frac{dM}{dt} = 0 \text{ and } C_{600} = C_0 \tag{7}$$

With another control volume cutting at x, another mass balance equation could be obtained:

$$\frac{dM}{dt} = C_0 q_m A - C_x q_m A + Re \tag{8}$$

So at steady-state C = C_0 over x.

In this case, we divided the control volume into two control volumes when the plume reaches a with the moving of the plume, then

$$\frac{dM}{dt} = C_0 q_m A - C_a q_m A \tag{9}$$

So we can get C = C_0 when x < a or x = a, and C = 0 when x > a.

For problems, where diffusion, dispersion, and reduction are negligible in comparison with advection, there are stationary vapor and solid phases with the moving bulk water along the x direction and the geometry is such that the problem can be treated as one-dimensional (Lundegard and Johnson, 2004), the GTE can be reduced from

$$\frac{\partial}{\partial t}(\phi_v C_v + \phi_m C_m + \rho C_s) = -\frac{\partial}{\partial x}(q_{m,x} C_m) + \frac{\partial}{\partial x}\left(D_m^{eff}\frac{\partial C_m}{\partial x} + \phi_m D_m^{diap}\frac{\partial C_m}{\partial x}\right) \tag{10}$$

to:

$$\frac{\partial}{\partial t}\{(\phi_v H + \phi_m + \rho K_s)C_m\} = -\frac{\partial}{\partial x}(q_{m,x} C_m) \tag{11}$$