



# Estimating the persistence of organic contaminants in indirect potable reuse systems using quantitative structure activity relationship (QSAR)

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## ABSTRACT

Predictions from the quantitative structure activity relationship (QSAR) model EPI Suite were modified to estimate the persistence of organic contaminants in indirect potable reuse systems. The modified prediction included the effects of sorption, biodegradation, and oxidation that may occur during sub-surface transport. A retardation factor was used to simulate the mobility of adsorbed compounds during sub-surface transport to a recovery well. A set of compounds with measured persistent properties during sub-surface transport was used to validate the results of the modifications to the predictions of EPI Suite. A comparison of the predicted values and measured values was done and the residual sum of the squares showed the importance of including oxidation and sorption. Sorption was the most important factor to include in predicting the fates of organic chemicals in the sub-surface environment.

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## 1. Introduction

Incomplete removal of pharmaceutical and personal care products (PPCPs) during wastewater treatment was first reported in the 1960s and subsequently, many reports of PPCPs in the aquatic environment have been published (Daughton and Ternes, 1999; Heberer, 2002; Kolpin et al., 2002; Stumm-Zollinger and Fair, 1965; Ternes, 1998). Although wastewater treatment plants (WWTPs) treat PPCPs using biological and/or physicochemical methods, most WWTPs release PPCPs and their metabolites into the aquatic environment at low concentrations (Heberer, 2002; Hirsch et al., 1999; Lam et al., 2004). Some investigators reported that the concentrations of PPCPs in WWTP effluents exceeded several micrograms per liter (Halling-Sørensen et al., 1998; Kolpin et al., 2002). The majority of PPCPs are completely mineralized to H<sub>2</sub>O and CO<sub>2</sub> or adsorbed to activated sludge in WWTPs (Daughton and Ternes, 1999; Ternes, 1998). However, persistent compounds not completely treated during wastewater treatment may be released to an aquatic environment where they are not easily degraded. Many persistent compounds are also readily adsorbed to solids in the soil due to their high hydrophobicity (Monteiro and Boxall, 2010). Even though the concentrations of these drugs are very low in the aquatic environment, their fates during the sub-surface transport have not been thoroughly investigated. Heberer (2002) reported that some of the PPCPs in WWTP effluents can affect groundwater quality due to their persistence in the aquifer. During studies of indirect potable reuse systems, most organic matter

including PPCPs can be transformed by microbial enzymes in the sub-surface environment providing sufficient surface area and travel time exist (Drewes et al., 2002, 2005; Fox et al., 2001).

The reuse of water for potable purposes is most commonly practiced by recharging groundwater with treated water and recovering the recharged groundwater with wells. This practice is termed indirect potable reuse since the recharged groundwater undergoes natural treatment processes and there is no direct connection between the wastewater treatment systems and the water distribution system. In general, there are two types of planned indirect potable reuse systems. One system uses spreading basins to recharge groundwater with wastewater treated by advanced secondary or tertiary treatment (Drewes et al., 2002; Fox et al., 2001). A schematic diagram of an indirect potable reuse system using spreading basins is shown in Fig. 1. As shown in Fig. 1, reclaimed water applied to a spreading basin will transport through both the vadose zone and the saturated zone and the retention time in the saturated zone may be months or years. Persistent compounds in reclaimed water may be transformed during sub-surface transport in the vadose zone and the saturated zone and these transformations are the primary removal mechanisms. The extracted water from the aquifer can be recovered for potable purposes. The second type of indirect potable reuse system uses advanced treatment processes such as reverse osmosis to treat water prior to injection into the ground using injection wells. Reverse osmosis eliminates most concerns over pharmaceuticals and other trace contaminants (Drewes et al., 2005). However, the fates of persistent compounds when spreading basins are used for indirect potable reuse are potentially of concern. This concern is difficult to address by monitoring alone and a predictive tool would be useful

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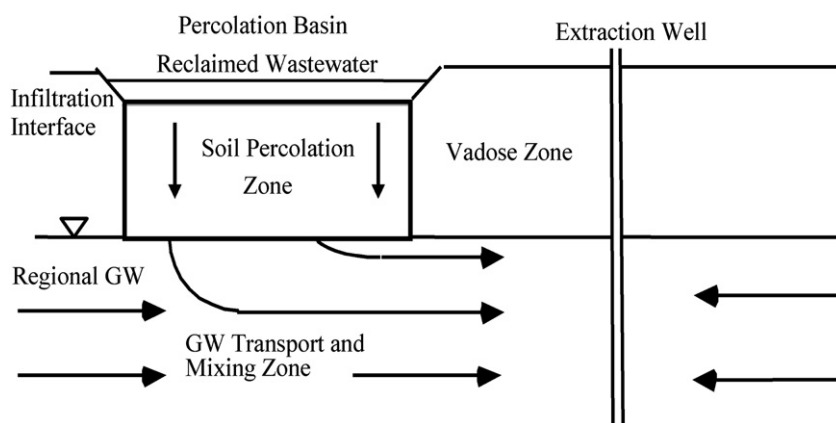


Fig. 1. A schematic diagram of soil aquifer treatment.

not only to reduce monitoring requirements but also to predict the fates of new organic compounds that may become widely used in the future.

The United States Environmental Protection Agency (US EPA) has several publicly available models to estimate persistence, bioaccumulation, and toxicity of organic chemicals in the environment. EPI Suite consists primarily of the two quantitative structure activity relationship (QSAR) models, the atmospheric oxidation program for Microsoft Windows (AOPWIN) and the biodegradation probability program for Microsoft Windows (BIOWIN), along with other QSAR models. Several investigators showed the accuracy of predictions by AOPWIN (Guesten et al., 1995; Sabljic and Peijnenburg, 2001). AOPWIN has been shown to provide precise predictions with approximately 90% accuracy for 500–600 organic compounds (Mackay and Boethling, 2000). BIOWIN was developed and improved starting in the 1980s to predict the potential for biodegradation of organic compounds in water and how the compounds will partition into soils and sediments using the Level III fugacity model (Boethling and Sabljic, 1989; Boethling et al., 1994; Howard et al., 1992; Mackey et al., 1992; Meylan et al., 2007; Tunkel et al., 2000). However, several investigators reported that EPI Suite and in particular BIOWIN had limited accuracy to predict the fates of organic chemicals (Aronson et al., 2006; Gouin et al., 2004; Kühne et al., 2006). Niederer and Goss (2008) found similar results to Kühne et al. (2006), however they stated that the quantitative structure property relationships of EPI Suite were not appropriate for all environments. The objective of this study was to modify the results from BIOWIN to more accurately estimate the fates of contaminants in indirect potable reuse systems. Of greatest concern is the removal of contaminants that persist after treatment in WWTPs and may be transformed during the sub-surface transport portion of indirect potable reuse systems. Improved accuracy will provide better agreement with existing studies and allow for the model to be used to analyze compounds that may be used widely in the future.

## 2. Methodology

### 2.1. Overview of compounds studied

The majority of work completed in this study was the development of a predictive model using the results from BIOWIN to better predict the fates of compounds during sub-surface transport in indirect potable reuse systems. Validation of the prediction was based on a group of 46 compounds studied by Westerhoff et al. (2005). These compounds were selected for study by Westerhoff et al. (2005) based on the criteria that their persistence was known, they represented a wide range of chemical structures and properties, and they were widely used. Of the 46 compounds studied by Westerhoff

et al. (2005), a literature search identified 35 compounds where half lives were measured under conditions similar to indirect potable reuse systems.

### 2.2. Modification of predictions from EPI Suite to estimate the persistence of organic chemicals in indirect potable reuse systems

EPI Suite is based on AOPWIN and BIOWIN and modification was necessary to get more accurate predictions for indirect potable reuse systems that involve sub-surface storage and transport. EPI Suite does not consider important environmental factors such as sorption or oxidation of compounds by co-metabolic reactions. In the sub-surface environment, organic chemicals may be strongly affected by adsorption because of the large interfacial surface area. BIOWIN predicts the biodegradability of a compound in water by calculating half life categories with values of 8.7, 15, 37.5, 60, and 180 days (US EPA, 2005). During sub-surface transport, sorption will effectively retard the movement of a compound. Strongly adsorbed compounds will not transport to a recovery well. While sorption can limit the bioavailability of a compound, if a compound is biodegradable it will have greater time for biodegradation since it is slowly released into the environment (Eberbach, 1998; Nam and Alexander, 1998).

The predicted half life from BIOWIN was first modified to include the effects of sorption. Bouwer (1991) reported that the retardation factor ( $R_f$ ) for a particular chemical species in the sub-surface is the ratio of solution velocity to species velocity. In other words,  $R_f$  implies the ratio of the rate of groundwater movement to that of contaminant movement. The mass fraction of a given compound (retarded contaminant) shows a positive relationship between hydrophobicity of a chemical and its accumulation on a solid. In this study, the sorption effects were simulated analogous to a retardation factor for sub-surface transport where the sorption limits the mobility of a compound to transport to a recovery well. The second modification was to include the potential for oxidation of compounds by cometabolism. One of the primary removal mechanisms for compounds at trace concentrations in indirect potable reuse systems is oxidation by cometabolic reactions (Nalinakumari et al., 2010; US EPA, 1998). This is because the concentrations of the compounds are too low to directly support the growth of microorganisms. When organic chemicals are cometabolized, oxygenases usually mediate the transformations. Given that microbial enzymes are involved in the biodegradation of organic chemicals and most cometabolic reactions are catalyzed by oxygenase enzymes when exogenous substrates are cometabolized, they are important for the long term transformation of compounds in indirect potable reuse systems (Bartels et al., 1984; Karuzina and Archakov, 1994). Since there is no QSAR model for these reactions, the general susceptibility to oxidation as predicted

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