Chapter 20

SOIL SORPTION COEFFICIENT

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ABSTRACT

Results for soil sorption coefficient K_{OC} are presented for 336 hydrocarbon and organic chemicals. The chemicals include hydrocarbon, oxygen, nitrogen, halogen, sulfur and phosphorus compounds. Representative results for soil adsorption coefficient [(mg sorbed / kg organic carbon in soil) / (mg/L aqueous concentration) or abbreviated as L/kg] are 4300 for trifluralin (C10H9F3N3O4), 3910 for hexachlorobenzene (C6CL6), 1300 for naphthalene (C10H8) and 27 for phenol (C6H6O) in a normal soil environment (20 C, pH 4-8, carbon exchange capacity greater than 7 MEQ/100 g, sand composition less than 70%, etc.). The melting point (MP) and molecular weight (MW) data are also provided as they are needed in many environmental property data correlations.

INTRODUCTION

The soil sorption coefficient K_{OC} , which determines the partitioning of an organic chemical between the soil/sediment and the aqueous solution, is an important environmental parameter. K_{OC} affects the physical movement of pollutants, chemical degradation (photolysis and hydrolysis), biodegradation, acidity and buffered solution-phase concentration. As a result, the soil sorption coefficient is widely used in river, runoff and soil/ground water models for the assessments of the fate and transport of chemicals (5,24,28,36). K_{OC} is also known as "soil organic carbon partition coefficient" or "soil sorption coefficient standardized with respect to organic carbon." With the value of K_{OC} known, the partition uptake of water contaminants for a particular soil/sediment or the degree of leaching of the pollutants into the ground water can be estimated.

A compilation of the soil sorption coefficient data for 336 compounds is provided in an easy-to-use tabular format that is especially applicable for rapid engineering use with the personal computer or hand calculator.

SOIL SORPTION COEFFICIENT

The amount of chemicals sorbed onto a soil or sediment depends on the concentration of chemicals and their equilibrium distribution coefficient (i.e., K_{OC}). For dilute aqueous solutions, the distribution coefficient can be adequately expressed with the Freundlich equation with 1/n equal to one (8,11,24,25,38):

$$x / m = K_{OC} C \tag{20-1}$$

where x = weight of solute sorbed, mg
C = equilibrium concentration of solute in aqueous phase, mg/L
m = weight of sorbent (organic carbon in soil), kg
K_{OC} = soil sorption coefficient

From the above equation, K_{OC} can be interpreted as the ratio of the solid phase concentration (normalized for the organic carbon content) to the solution phase concentration of the chemical at equilibrium. Therefore, in commonly used units, K_{OC} is:

$$K_{OC} = \frac{\text{mg sorbed/ kg organic carbon}}{\text{mg/L aqueous concentration}} \tag{20-2}$$

The unit of K_{OC} can be abbreviated as L/kg. The average organic carbon content of a typical soil is from 0.5% to 3.5%. By basing the sorption coefficient on soil (or sediment) organic carbon, one can eliminate much of the variation between soils due to organic carbon content. Note that the cited experimental or predicted K_{OC} values are intended for a normal environment as stated above. Attempts to extrapolate far beyond these conditions may incur considerable errors (10-12,15,24). In case that the coefficient is expressed in terms of soil organic matter, K_{om}, the following equivalence can be used to obtain K_{OC}:

$$K_{OC} = 1.72\ K_{om} \tag{20-3}$$

This assumes that the organic matter contains about 58% C (8).

The results for the soil sorption coefficient for organic chemicals in water are given in Table 20-

1. The melting point (MP) and molecular weight (MW) are also provided to facilitate predictions for other
environmental properties. The tabulation is applicable to a wide variety of organic chemicals in contact with water at normal ambient conditions. The wide variety of substances includes hydrocarbons, acids, alcohols, esters, ethers, ketones, fluorides, chlorides, bromides, amines, sulfones, nitros, amides, sulfides and phosphates. The tabulation is arranged by carbon number (C, C2, C3, ... C21). This provides ease of use in quickly locating data using the chemical formula.

In preparing the tabulation, a literature search was conducted to identify data source publications (1-40). The publications were screened and copies of appropriate data were made. These data were then keyed into the computer to provide a database.

The nonlinear group contribution method (3,13,21) has been used for the estimation of the soil sorption coefficient when experimental K_{OC} values are not available. The method is based on comprehensive (225 compounds) and updated data. Comparison with literature methods yields favorable results (2,3,13,19,32,33). In general, the prediction errors are within ± 0.82 order of magnitude (95% confidence limit). A comparison of calculated and data (experimental) values for the soil sorption coefficient is shown in Figure 20-1. The graph discloses general agreement of calculated and data values for different organic chemicals.

The compilation for the soil sorption coefficient maybe used in engineering and environmental impact studies involving organic compounds in water.

EXAMPLES

The tabulation may be used for determining the soil sorption coefficient for the compound in water. The use of the soil sorption coefficient in environmental applications involving organic chemicals in water is illustrated below.

Example 1 For an aqueous concentration of benzene (C6H6) in contaminated river water of 10 ppm by weight, what will be the maximum uptake of benzene by the bottom sediment? The average organic carbon content of the bottom sediment is 3%.

The equation x/m = K_{OC} C is used in determining the solution. First, calculate the amount of organic carbon per ton (metric) of bottom sediment: m = 1000 * 3% = 30 kg organic carbon. Then substitute the soil sorption coefficient of benzene from the tabulation

K_{OC} = 83 (mg sorbed/kg org carbon) / (mg/L aqueous conc) = 83 (mg sorbed/kg org carbon) / (ppm aqueous conc)

and the aqueous concentration C = 10 ppm into the equation for x/m to obtain:

x /30 = 83 * 10 mg

x = 30*83*10 mg = 2.5E04 mg = 0.025 kg

Example 2 Atrazine (C8H14CLN5) is uniformly applied to a field and incorporated into the soil. The soil has a bulk density of 1.25 kg/L, 2 % organic carbon and 25 % each air and water by volume. Estimate the equilibrium distribution of the pesticide resulting from a 1 kg/hectare (1 hectare = 10,000 m^2) application incorporated to 10-cm depth. Volatilization into the air is assumed to be negligible.

The amount of organic carbon in soil per hectare is m = 10,000 *.1 * 1000 * 1.25 * 2% = 25,000 kg of org carbon. From the tabulation, the soil sorption coefficient of atrazine is

K_{OC} = 149 (mg sorbed/kg organic carbon) / (mg/L aqueous conc)

Determination of the amount of atrazine in the soil phase per hectare requires a trial and error procedure. Trying x = .94 kg = 940000 mg in the equation x/m = K_{OC} C and solving for C gives:

C = (940000 /25,000)/149 = .252 mg/L

The amount of atrazine in the aqueous phase per hectare is

.252 * 10,000 * .1 * 1,000 * 25% = 63000 mg = .063 kg

The total amount of atrazine is 1.003 kg/hectare. This is close enough to the application (1.003 vs 1 application).

The equilibrium distribution of atrazine is estimated to be:

.063/(.94 + .063) = 6.3 % in water

.94/ (.94 + .063) = 93.7 % in soil

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