Standard Test Method for
Determining a Sorption Constant (K_{oc}) for an Organic Chemical in Soil and Sediments[1]

This standard is issued under the fixed designation E 1195; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This test method describes a procedure for determining the partitioning of organic chemicals between water and soil or sediment. The goal is to obtain a single value which can be used to predict partitioning under a variety of environmental conditions from the measurement of sorption coefficients for specific solids.

1.2 Sorption represents the binding process of chemicals to surfaces of soils or sediments through chemical, or physical, or both interactions.

1.3 The sorption of nonpolar organic chemicals, and to some extent polar organic chemicals, is correlated with the organic carbon content of the sorbing solid. Charged inorganic and organic molecules may behave differently, and some other property, such as, cation exchange capacity, clay content, or total surface area of sorbing solids, may influence sorption. Hydrous metal oxides of iron and aluminum may significantly affect sorption in sediments. In order to provide a sorption coefficient that is useful for a wide range of soils and sediments, the coefficient is based on organic carbon content. This approach, however, will not apply to all chemicals or all soils and sediments. In cases where it does not apply, the investigator may need to seek other methods of relating sorption to the properties of the chemical, soil, or sediment.

1.4 It is possible that, in addition to organic carbon, sorption is correlated with the total surface area of sorbing solids. This may be particularly important with solids having organic carbon contents so low that sorption to inorganic surfaces is significant in comparison to sorption by organic material. In such a case, inclusion of the total surface area into the sorption calculation may be useful. For further information on this subject see Ref (**1**).[2]

1.5 Equilibrium sorption coefficients are determined. It is recognized that equilibrium conditions do not always exist in environmental situations, but sorption equilibria values are necessary for making generalizations about environmental partitioning.

1.6 Studies are conducted preferably with an analytical or technical-grade chemical. Mixtures are used only if analytical methods allow measurement of individual components of interest in the mixture. Good laboratory procedures must be followed to ensure validity of the data.

1.7 *This standard does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*
D 421 Practice for Dry Preparation of Soil Samples for Particle-Size Analysis and Determination of Soil Constants[3]
D 422 Test Method for Particle-Size Analysis of Soils[3]
D 1193 Specification for Reagent Water[4]
D 4129 Test Method for Total and Organic Carbon in Water by Oxidation Coulometric Detection[5]
2.2 *Other standards:*
OECD Test Guideline 106[6]

3. Terminology Definitions

3.1 *sorption distribution coefficient* (K_d)—the concentration of chemical sorbed by solids, in µg/g, on an oven-dry solids weight basis divided by the concentration of chemical in the water, in µg/g, at equilibrium.

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[1] This test method is under the jurisdiction of ASTM Committee E47 on Biological Effects and Environmental Fate and is the direct responsibility of Subcommittee E47.04 on Environmental Fate of Chemical Substances.
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[2] The boldface numbers in parentheses refer to the list of references at the end of this test method.

[3] *Annual Book of ASTM Standards*, Vol 04.08.
[4] *Annual Book of ASTM Standards*, Vol 11.01.
[5] *Annual Book of ASTM Standards*, Vol 11.02.
[6] Available from the Organization for Economic Co-Operation and Delevopment 2, rue André Pascal F-75775 Paris Cedex 16 France.

3.2 *organic carbon normalized sorption constant (K_{oc})*—the sorption distribution coefficient, K_d, normalized to the relative organic carbon content (fraction) of the solid oc ($K_{oc} = [k_d/\%OC] \times 100$).

4. Summary of Test Method

4.1 The sorption coefficient of a chemical is measured by equilibrating an aqueous solution containing an environmentally realistic concentration of the chemical with a known quantity of soil or sediment. After reaching equilibrium, the distribution of chemical between the water and the solids is measured by a suitable analytical method. If appropriate for the test material, sorption constants are calculated on the basis of the organic carbon content of the solids. In addition to reporting single values for each solid, the sorption constants from all solids are averaged and reported as a single value.

5. Significance and Use

5.1 Sorption data are useful for evaluating the migratory tendency of chemicals into the air, water, and soil compartments of our environment. They can be used in the prediction or estimation of volatility from water and soil, concentration in water, leaching through the soil profile, run-off from land surfaces into natural waters, and biological availability. Additional information concerning testing to determine sorption coefficients can be found in OECD test Guide 106 (**7**).

5.2 This test method assumes that sorption of at least nonpolar organic chemicals is mainly influenced by the organic matter of the soil or sediment solids. There is ample evidence in the literature to support this assumption, and the user of this test method should refer to Ref. (**2**) for more information on this subject. Organic *carbon* content is chosen as the basis for sorption instead of organic *matter* content. This is because organic carbon values generally are measured directly by analytical methods. Organic matter may be estimated by multiplication of the organic carbon values by a somewhat arbitrary constant of 1.7 (**3**). This test method is based on the assumption that all of the material sorbed to the solids is reversibly bound. The analyses described herein assume equilibrium between the liquid and solid concentrations of the test compound. In some cases, there may be a fraction of the compound that is irreversibly bound to the solids. For these cases, the measurements made by the test may not reflect a true "equilibrium". The irreversible sorption phenomena has been extensively documented and the reader is referred to (**9**), (**10**) and (**8**) for more discussion on this topic.

5.3 A sorption constant is obtained and is essentially independent of soil properties other than organic carbon. This value is useful because, once it is determined, the sorption distribution characteristics for any solid can be estimated based on its organic carbon content.

5.4 This test method is designed to evaluate sorption at environmentally relevant concentrations as a function of organic carbon content of different soil and sediment solids. Therefore, the number of different solids is emphasized in the procedure rather than the number of chemical concentrations studied with each solid. In general, one concentration is employed since the test method assumes that at low solution concentrations, sorption isotherms approximate linearity and sorbed concentrations do not exceed typical environmental loading. Errors arising from concentration effects at low environmental concentrations usually are less than the variation existing between different solids, when dealing with sorption trends in a general manner. Therefore, the initial concentration of the test chemical in solution should not exceed 0.5 of its water solubility.

5.5 As an option, a procedure is given for determining concentration effects on sorption. This is because high concentrations may be present in certain environmental situations; such as landfills and spills. This procedure should be done at four concentrations over a hundred fold concentration range (for example, 0.1, 0.5, 2, and 10 ppm initial solution concentration). If low solubility presents analytical difficulties, solution concentrations should range over at least one order of magnitude. The Freundlich equation is an appropriate expression of these effects:

$$C_a = KC_s^{1/n} \tag{1}$$

where:
C_a = chemical adsorbed, oven-dry solids weight, µg/g,
K = sorption coefficient,
C_s = solution concentration at equilibrium, µg/g, and
$1/n$ = exponent.

5.5.1 A log plot of the Freundlich equation yields the following linear relationship:

$$\log C_a = \log K + 1/n \log C_s \tag{2}$$

6. Apparatus

6.1 *High-Speed Temperature Controlled Centrifuge*, capable of removing particles 0.1-µm radius from solution. Details of centrifugation techniques are given in the Procedure section.

6.2 *Centrifuge Tubes*, capable of withstanding high speed and made of glass, metal, or other suitable material which minimizes adsorption of the test chemical to its surface. The tubes should be capped with TFE-fluorocarbon or aluminum-lined screw caps.

6.3 *Analytical Instrumentation*, suitable for measuring the concentration of the test chemical in solids and water.

6.4 *Laboratory Oven*, capable of maintaining a temperature of 103 to 110°C. The oven is used for determining the moisture content of soils or sediments.

7. Reagents and Materials

7.1 Analytical or technical grade chemical of known purity should be used. If available, all reagents shall conform to the specifications of the Committee on Analytical Reagents of the American Chemical Society.[7] Radiolabeled test materials of known radio-purity or nonlabeled test materials of known composition are suggested.

7.2 *Purity of Water*—Reagent water shall conform to Specification D 1193 for Type IV grade water.

8. Sampling, Test Specimens, and Test Units

8.1 Use soils or sediments, or both, varying in organic carbon content, pH, and texture or particle-size distribution. Four to seven different samples are recommended. Record their history, if available, description, and site location.

8.2 Collect soil samples in containers lined with polyethylene bags. Collect from the top 6 in. of the soil profile and before storing, screen through a 2-mm sieve. Store at 4°C. Store and handle the soil samples at the moisture content at time of collection. If initial moisture content is too high for satisfactory screening, partially dry the soil samples, by exposing to air for brief periods. When using air-dried soil samples, longer sorption equilibrium times may be required to allow the organic matter to become thoroughly wetted.

8.2.1 Determine the soil pH, particle-size distribution, and organic carbon content for each soil sample. Cation or anion exchange capacity may be needed for charged molecules. Refer to Ref **(3)** for measurement methods.

8.2.2 Determine the moisture content on a soil specimen allowing sorption to be based on oven-dried solids weight. Discard the soil specimen after determining the moisture content.

8.3 Sediment samples from aquatic systems should not be air-dried or frozen prior to use. Collect sediment samples with a suitable grab or coring device and, if not used immediately, store in a suitable bottle at 4°C for periods up to 10 days. Minimal sediment characterization should include organic carbon content and particle-size distribution. Work with ions and molecules having functional groups capable of ionizing can be aided by characterization of redox potential, pH, and cation or anion exchange capacity of the sediments.

8.3.1 Measurement of sorption properties of anoxic sediments, usually characterized by the presence of a hydrogen sulfide odor, requires strict adherence to oxygen exclusion during a test. Admission of even small amounts of oxygen to the diluted sediments suspension will allow oxidation of ferrous iron with a concomitant precipitation of ferric hydroxide, which is a highly efficient scavenger for many dissolved constituents. However, when the primary area of concern in the aquatic system is aerobic, conduct the test under a normal air atmosphere using well-aerated sediments. For further information consult Ref **(4)**.

8.4 Base the solids content (or conversely, water content) of the soil or sediment specimen on the oven-dry weight (24 h drying at 103 to 110°C). Only in the case of very dilute sediment suspensions (0.1 % solids or less) are dry-weight corrections for dissolved inorganic and organic species required. Do not reuse in any sorption measurement the specimens used for this dry-weight solids determination.

8.5 Combustion is the preferred measurement method for organic carbon, using the procedures described in Test Method D 4129 or other similar procedures.

8.6 Determine the particle-size distribution by a combination of sieving and sedimentation. The fractions are gravel (>2 mm), sand (2.0 to 0.05 mm), silt (0.05 to 0.002 mm), and clay (<0.002 mm). Refer to Ref. **(3)**, Practice D 421, and Test Method D 422 for a description of this procedure.

8.7 Measure the soil or sediment specimen pH using a 1:1 soil slurry procedure **(3)**. Stir the suspension several times over a 30-min period and allow to stand 1 h. Then measure the pH of the supernatant fluid above the soil suspension.

8.8 Prepare a test chemical water solution by dissolving the chemical in water. Make sure the test concentration is below water solubility and, preferably, near concentrations expected in the environment. Unless otherwise indicated, references to water shall be Type IV reagent water. Care should be taken with volatile chemicals to minimize losses.

8.8.1 For those chemicals with water solubilities in the range of 0.1µ g/g or less, prepare a stock solution using acetonitrile or other appropriate solvent miscible with water. Directly add the chemical to the solids and water system with 0.1 % or less volume of the cosolvent. If using this method, use the cosolvent at the same concentration in all tests.

9. Procedure

9.1 Conduct a preliminary study with one or more soil samples to determine, (*1*) the proper solids to water ratio to employ, (*2*) the amount of equilibration time required and, (*3*) whether sufficient decomposition or losses of the chemical takes place to require that both solids and water be analyzed in the main study. Methods for the preliminary study and the main study are the same, except where noted in the remainder of this section.

9.2 *First Estimate of K_{oc}*—Estimate the value of K_{oc} from the test compound water solubility. This estimate will aid in the selection of a solids to water ratio and will allow a statistically valid measurement concentration change in the water after sorption has taken place (see section on Selection of Water to Solids Ratios). Use the following equation to estimate the relationship between the measured K_{oc} values and water solubilities:

$$ln\ K_{oc} = (-ln\ W_s - 0.01\ (MP-25) + 15.1621)/1.7288 \qquad (3)$$

where:
W_s = water solubility, mg/L, and
MP = melting point, °C (for liquids at 25°C, MP = 25).

This equation predicts K_{oc} values within an order of magnitude.

9.2.1 Obtain estimates of K_d values for soils under investigation by multiplying the K_{oc} estimate by the percent organic carbon divided by 100. Use this estimate to select the appropriate solids to water ratio (see section on Selection of Water to Solids Ratios). If the K_d measured in the preliminary study is significantly different from the estimated value, use the measured value to estimate the solids to water ratios for the remaining soils or sediments of the main study.

9.3 After deciding upon the proper solids to water ratios, add aliquots of an aqueous solution of the test chemical to duplicate samples of pre-weighed soil or sediment (or volume of sediment suspension containing a known solids content).

9.4 Prepare duplicate aqueous samples, as described in 9.3, containing no solids. These serve as controls to correct for adsorption onto the surfaces of the centrifuge tube and cap. If surface adsorption is substantial, try centrifuge tubes of a different material to minimize this effect.

9.5 Prepare duplicate blanks containing water and solids, but no chemical, as described in 9.3 These serve as background controls during analysis to detect interfering compounds or contaminated soils.

9.6 Cap all samples with screw caps immediately after addition of solution and shake each continuously in the dark so that good mixing occurs during equilibration. Select a shaker that will provide enough agitation to keep most of the solids in suspension.

9.7 The time required for sorption equilibrium in the soil or sediment samples is highly variable, depending on the chemical and the sorbent (5). Therefore, in the preliminary study, four sets of duplicate samples are sampled sequentially over a 48-h period of mixing (for example, 4, 8, 24, 48 h). A suitable equilibration time is selected for use in the main study.

9.8 Centrifuge the samples, at 25°C, at a speed fast enough and for a sufficient time period to remove particles 0.1-μm radius from the solution. This is particularly important for highly sorbed chemicals because significant error could result if most of the chemical in the water was adsorbed to particles not removed by centrifugation. Centrifugation conditions will vary from one instrument to another, but can be calculated from Stokes Law (see Calculations section).

9.9 In the preliminary study, analyze both the water and solids phases for test chemical and perform a mass balance in comparison with control samples. This procedure is very important for volatile chemicals as they can be lost from the test systems. In the case of volatile chemicals, it is recommended that a system mass balance be determined to assess chemical losses. If decomposition is noted or if a mass balance less than 90 % is obtained, analyze both phases in the main study. If this is not the case, calculate the amount of chemical sorbed to solids from the concentration change observed in the water between the control samples and the samples containing solids.

10. Selection of Water to Solids Ratios

10.1 Selection of appropriate water to soil ratios for sorption studies will depend on the sorption coefficient (K_d) and the relative degree of sorption desired. The degree of sorption of chemical from solution will determine the statistical accuracy of the measurement based on the form of the sorption equation and the limit of the analytical methodology in detecting the concentration of the chemical in solution.

10.2 Consider the sorption equation:

$$K_d = \frac{\mu g s \text{ chemical/g solids}}{\mu g w \text{ chemical/g } H_2O} \qquad (4)$$

where:
K_d = sorption coefficient,
$\mu g s$ = chemical sorbed, μg,
$\mu g w$ = chemical in solution at equilibrium, μg, and
S = g solids/g water.

This can be rearranged to obtain:

$$K_d = \frac{\mu g s}{\mu g w} \left(\frac{1}{S}\right) \qquad (5)$$

And applying the material balance equation:

$$\mu g w^0 = \mu g w + \mu g s \qquad (6)$$

where $\mu g w^0$ = total μg initially in solution.
One obtains:

$$K_d = \frac{\mu g s}{\mu g w^0 - \mu g s} \left(\frac{1}{S}\right) \qquad (7)$$

For example, if solids to water ratio is 1:5, $S = 0.2$, and if 20 % of the chemical is sorbed ($\mu g s / \mu g w = 0.2$), then, from (Eq 7), $K_d = 1.25$.
By arranging (Eq 7) to the form of (Eq 8),

$$\frac{\mu g s}{\mu g w^0} = \frac{K_d S}{1 + K_d S} \qquad (8)$$

one can construct plots of percent sorbed ($\mu g s / \mu g w \times 100$) versus K_d. Such plots are shown in Fig. 1 for 2:1, 5:1, 20:1, 100:1, and 1000:1 water to solids ratios. Two aspects of these plots become apparent. (1) At a specific ratio, as percent sorbed increases, a small change in this value can result in a rather large change in K_d. This is particularly true above 80 % sorbed. (2) As K_d becomes very small, percent sorbed decreases rapidly, such that measurements in these cases needed to be made at as low as possible water to solids ratio. Therefore, in general, it is most desirable to be between 20 and 80 % sorbed. This is possible by selection of the appropriate water to soil ratio based on an estimate of the value of K_d either by preliminary studies or by established estimation techniques. Selection of an appropriate ratio can then be made based on a
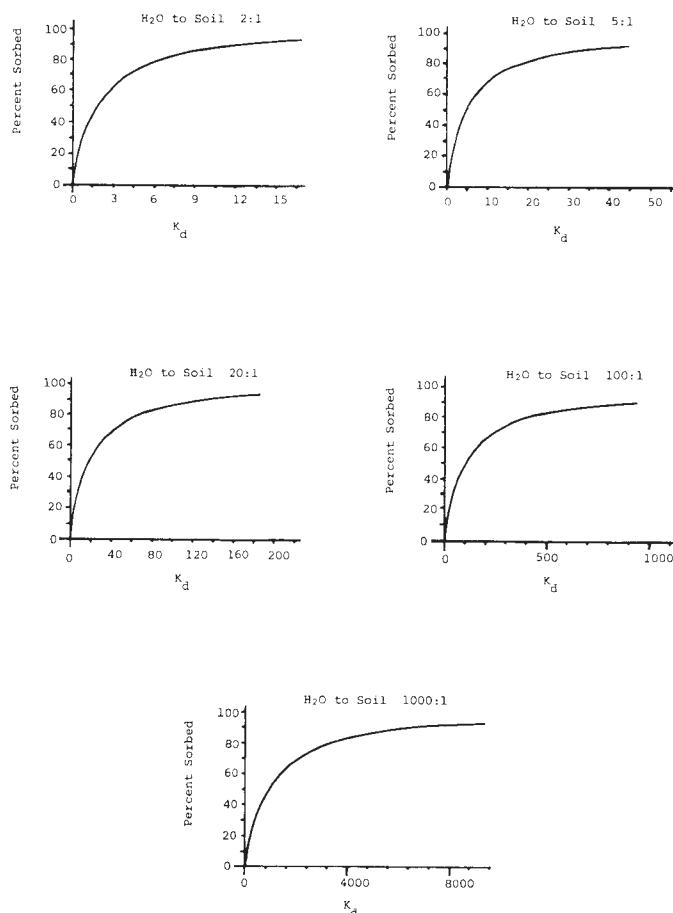

FIG. 1 Relationship Between Percentage Sorbed and K_d at Various Ratios of Water to Soil Solids

plot of water to solids ratio (1:*S*) versus K_d for fixed percentages of sorbed material. The applicable relationship is obtained by re-arranging (Eq 7) to the form of (Eq 9).

$$\frac{1}{S} = \left(\frac{\mu g w^0}{\mu g s} - 1 \right) \times K_d \qquad (9)$$

10.3 Fig. 2 shows the water to solids ratio (l:*S*) required as a function of K_d for 90, 70, 50, 30, and 10 % sorption. For example, with a water to solids ratio of 5:1 and a K_d of 12.5, approximately 70 % sorption would occur, which would fall within acceptable limits. To obtain 50 % sorption for the same K_d a 12.5:1 ratio would be used.

10.4 Ideally, sorption studies can be made at any water to solids ratio, but in practice it is perhaps useful to standardize on a few fixed ratios, as long as the percent sorbed falls within 20 to 80 %. Use of ratios 5:1, 20:1, and 100:1 is recommended. These ratios will cover the 20 to 80 % sorption ranges for K_d values of approximately 1 to 20, 4 to 80, and 20 to 400, respectively. This should give each investigator the flexibility to meet experimental needs.
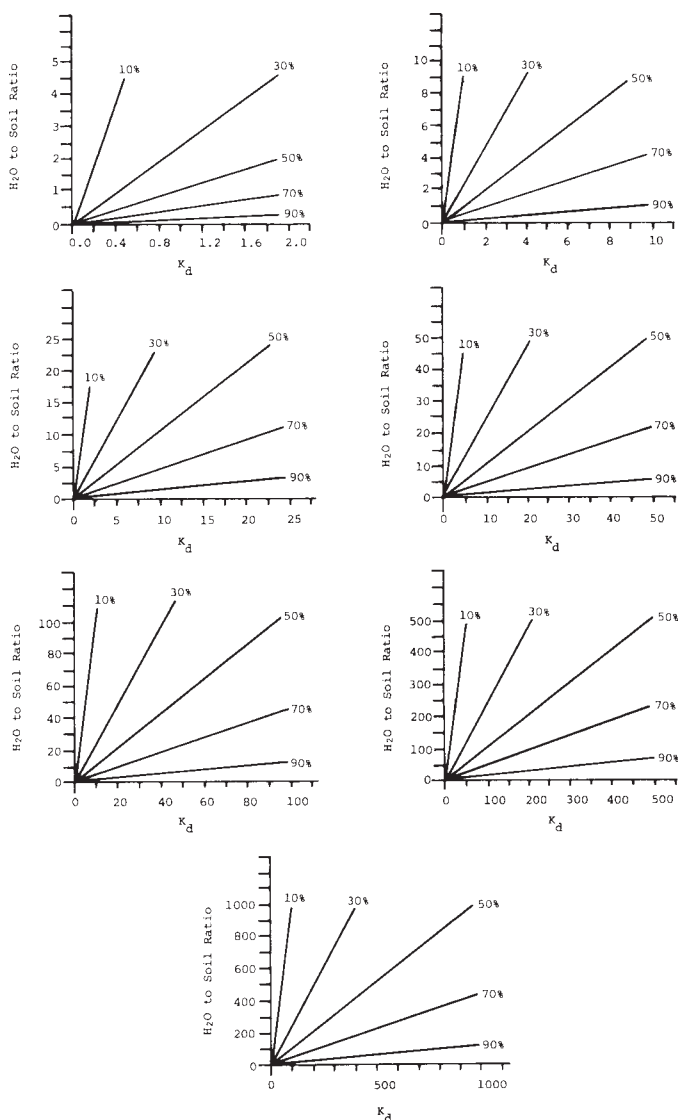
10.5 Areas which are more difficult to deal with are those where the chemical is very highly or very slightly sorbed. Where low sorption occurs, a 2:1 water to solids ratio should be used. Care must be taken with the analytical methodology to measure small changes in solution concentration. Alternatively, at very high sorption coefficients, one can go to a 1000:1 water to solids ratio to leave a significant amount of chemical in solution. However, care must be taken to ensure good mixing and adequate time must be allowed for the system to equilibrate. It is recommended that at least 0.5 g of soil be used, preferably 1 g. Therefore samples will consist of 500 to 1000 mL of solution. In cases where only the water is being analyzed and the amount of chemical sorbed is calculated by difference, only aliquots of the solution need be centrifuged for analysis.

11. Calculation

11.1 Centrifuge time to remove particles >0.1-μm radius and 2.65-g/cm³ density from solution:

$$t = \frac{2.22 \times 10^{10}}{(r/\min)} \ln R_b/R_t \qquad (10)$$

where:
t = seconds,
$r/\min$ = revolutions per minute,
R_t = distance from center of centrifuge rotor to top of solution in centrifuge tube, cm, and
R_b = distance from center of centrifuge rotor to bottom of centrifuge tube, cm.

11.2 This assumes spherical particles and:

$$t = 9/2 \left[\frac{n}{\omega^2 r_p^2 (\rho_p - \rho)} \right] \ln (R_b/R_t) \qquad (11)$$

where:
ω^2 = $\dfrac{4\pi^2 (r/\min)}{3600}$,
r_p = particle radius = 1×10^{-5} cm,
n = viscosity of water at 25°C = 8.95×10^{-3} g/s cm,
ρ_p = particle density = 2.65 g/cm³, and
ρ = density of water = 1.0 g/cm³.

In general practice double the calculated times to ensure complete separation.

11.3 Moisture percentage of solids:

$$M = \frac{(A - B)\,100}{B} \qquad (12)$$

where:
M = moisture percentage,
A = sample wet weight, g, and
B = sample oven-dry weight, g.

11.4 Oven-dry solids weight in wet solids sample:

$$B = \frac{A}{1 + M/100} \qquad (13)$$

where:
B = oven-dry solids weight, g,
A = sample wet weight, g, and
M = moisture percentage.

11.5 Total water present:

$$W_T = W_A + (A - B) \qquad (14)$$

FIG. 2 Relationship Between Water to Soil Ratios and K_d at Various Percentages of Sorbed Material

where:
W_T = total quantity of water, mL,
W_A = volume of water added, mL,
A = wet weight of solids, g, and
B = oven-dry weight of solids, g.

11.6 Total chemical in water:

$$T = (W_T)(C_S) \quad (15)$$

where:
T = total quantity of chemical left in water, μg,
W_T = total quantity of water, mL, and
C_s = concentration of chemical in water, μg/mL.

11.7 Total chemical in solids (no breakdown):

$$G_S = G_A - T \quad (16)$$

where:
G_S = total quantity of chemical sorbed to solids, μg,
G_A = total quantity of chemical in control sample, μg, and
T = total quantity of chemical left in water, μg.

11.8 Calculation of sorption coefficient (K_d):

$$K_d = \frac{G_S/B}{C_s} \quad (17)$$

where:
K_d = sorption coefficient,
G_S = total quantity of chemical sorbed to solids, μg,
B = oven-dry weight of solids, g, and
C_s = concentration of chemical in water at sorption equilibrium, μg/mL.

11.9 Calculation of sorption coefficient (K) and $1/n$ using Freundlich equation for concentration study:

$$\log C_a = \log K + 1/n \log C_s \quad (18)$$

where:
K = sorption coefficient,
C_a = concentration of chemical in solids at equilibrium, μg/g (G_s/B),

C_s = concentration of chemical in solution at equilibrium, μg/mL, and
$1/n$ = exponent.

A plot of log C_a versus log C_s is constructed where:

$$1n = \text{slope and } \log K = \text{intercept} \quad (19)$$

11.10 Calculation of organic carbon normalized sorption constant (K_{oc}):

$$K_{oc} = \frac{K_d \times 100}{\% \ OC} \quad (20)$$

where:
K_{oc} = organic carbon normalized sorption constant,
K_d = sorption distribution coefficient, and
$\% \ OC$ = percentage of organic carbon in solids.

11.11 Then, average the sorption constants for the different soil samples to determine a mean K_{oc} value, the standard deviation, and the coefficient of variation.

12. Precision and Bias

12.1 An interlaboratory test program of this test method was conducted at four laboratories using trifluralin and 13 soil types. Each laboratory used two to four soil types, differing in each laboratory. The percent organic carbon of each soil type, sorption coefficient, and organic carbon normalized sorption constant are given in Table 1. If one soil (No. **8**) is excluded from the mean, the correction of sorption data for organic carbon content reduces the variability from 69 to 38 % in this particular study. In general, one can probably anticipate variations of 20 to 50 % of the mean K_{oc} value. This may seem like a large variation, but it is actually small with respect to the range of K_{oc} values covered by chemicals. This range is from zero to more than 10^5.

13. Keywords

13.1 equilibrium sorption coefficients; partitioning of organic chemicals; sorption constant (K_{oc})

TABLE 1 Sorption of Trifluralin by Thirteen Soils from Interlaboratory Study

Soil	Organic Carbon,%	K_d	K_{oc}
1	0.41	15.5	3 750
2	0.52	37.7	7 250
3	0.70	17.0	2 400
4	0.73	35.6	4 870
5	0.77	19.5	2 540
6	1.07	66.7	6 230
7	1.40	130.0	9 300
8	1.80	270.0	14 990
9	1.84	139.0	7 590
10	1.96	155.0	7 900
11	2.00	130.0	6 500
12	2.60	150.0	5 770
13	3.37	158.0	4 710
Mean		101.8	6 450
S_D		76.7	3 300
Coefficient Variation		75.3 %	51.1 %
Excluding Soil No. 8			
Mean		87.8	5 730
S_D		60.4 %	2 150
Coefficient Variation		68.7 %	37.6 %

APPENDIXES

(Nonmandatory Information)

X1. Ranking Sorption Tendencies

X1.1 The K_{oc} value of a chemical obtained from this test method represents a single value which characterizes the partitioning of a chemical between soils or sediments and water. This value then can be used in the evaluation of the fate and behavior of the chemical in the environment. It represents a parameter which is essentially independent of soil properties, such that a basis is established for ranking and comparing chemicals with respect to their soil to water partitioning tendencies. An example of such a ranking is given in Table X1.1.

TABLE X1.1 Sorption Constants for Several Chemicals

Chemical	K_{oc}
Dicamba	0
Cis 1,3-dichloropropene	26
Ethylene dibromide	32
Monuron	83
DBCP	130
Atrazine	170
EPTO	280
Nitrapyrin	460
Lindane	735
Trifluralin	4 300
Parathion	4 800
Chlorpyrifos	6 100
DDT	150 000

X2. Soil Mobility

X2.1 This process enables one to classify particular aspects of chemical behavior regarding various environmental transport processes. For example, the K_{oc} value represents an expression of the inherent mobility of chemicals in soil. Chemicals which have a low K_{oc} value are weakly sorbed and are therefore more mobile in soil. A mobility classification scheme based on K_{oc} values is given in the Table X2.1.

TABLE X2.1 Recommended Classification of Soil Mobility Potential of Chemicals

K_{oc}	Mobility Class
0–50	very high
50–150	high
150–500	medium
500–2000	low
2000–5000	slight
5000	immobile

X3. Sorption Effects on Volatilization

X3.1 Volatility of chemicals from soils or aquatic systems is modified by the sorption characteristics of the compound. If two chemicals have the same tendency to volatilize from a simple water environment, the one which is sorbed the least will demonstrate the highest potential for volatility transport in an environmental situation where soil or sediment is also present (for example a pond or a field). This is simply a result of the sorption process modifying the concentration of the chemical in the aqueous phase and in turn modifying the volatility characteristics of the compound (6).

X4. Mathematical Models for Chemical Fate Estimates

X4.1 In addition, the K_{oc} value is easily utilized in environmental modeling systems which combine all the environmental parameters that effect the fate of chemicals in the environment. For differing amounts of organic carbon selected to represent model systems, fairly reliable estimates of K_d can be obtained from the K_{oc} value and used in the modeling process. Therefore, this type of measurement can be extremely useful in evaluating expected distribution patterns of chemicals in the environment.

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