



SITE-SPECIFIC DISTRIBUTION COEFFICIENTS FOR PRELIMINARY MODELING PURPOSES

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ABSTRACT

Work was performed to generate site-specific distribution coefficient (K_d) values for possible use in groundwater modeling at two different landfill sites (denoted herein as Site 1 and Site 2) for an electric utility. While such coefficients are applicable only for the conditions under which they are generated, they are nonetheless useful in making preliminary assessments. Batch sorption experiments were conducted in consistence with procedures described by the U.S. Environmental Protection Agency. Twenty different soil samples were mixed and shaken with aqueous concentrations of constituents determined to be of concern, namely, arsenic (As), barium (Ba), boron (B), cadmium (Cd), chromium (Cr), fluoride (F), lead (Pb), mercury (Hg), nickel (Ni), selenium (Se), silver (Ag) and sulfate (SO_4). Three soil to solution ratios were investigated with 50 mL polystyrene tubes: 1:5, 1:50 and 1:500. These ratios were sufficient to produce measurable K_d values for virtually all soil samples and contaminants of concern. For Site 1, boron shows the least adsorption ($0 \text{ mL/g} < K_d < 3.75 \text{ mL/g}$) while fluoride shows the highest ($64 \text{ mL/g} < K_d < 1,167 \text{ mL/g}$). Similarly, for Site 2, boron also shows the least adsorption ($0.19 \text{ mL/g} < K_d < 4.98 \text{ mL/g}$) while lead shows the highest ($K_d > 1000 \text{ mL/g}$). Specific distribution coefficients for each contaminant and soil sample are presented with the primary purpose of contributing to the global database.

Key words: Sorption, Contaminant Transport, Fly Ash, Landfills.

INTRODUCTION

Batch sorption experiments are used to approximate the equilibrium relationship between aqueous and solid-phase (soil) concentrations of chemical contaminants. One of the main reasons for performing batch sorption tests is to determine the value of the distribution coefficient, K_d , which can then be incorporated into contaminant transport codes. While there are limitations to this approach, including the assumption of local equilibrium, uncertainty between lab and field conditions, etc., useful predictions can be made with K_d terms. Typically there is interest in computing the concentration of a given contaminant as a function of time or space.

Contaminant transport through materials may be described by the well-known partial differential equation which accounts for advection, dispersion and retardation (ADRE), given by:

$$\frac{\partial C}{\partial t} = \frac{D}{R} \cdot \frac{\partial^2 C}{\partial x^2} - \frac{v_s}{R} \frac{\partial C}{\partial x} \quad (1)$$

Where:

- C = solute concentration, (M/L³)
- t = elapsed time, (T)
- D = soil dispersion coefficient, (L²/T)
- x = curvilinear length in the direction of flow, (L)
- v_s = seepage velocity, (L/T)
- R = retardation coefficient, (dimensionless)

The retardation factor makes use of the experimentally-determined K_d, and is computed by:

$$R = \frac{v_s}{v_c} = 1 + \left(\frac{\rho_d}{n} \right) K_d \quad (2)$$

Where:

- v_c = contaminant velocity, (L/T)
- K_d = distribution of contaminant between solid and liquid phase, (L³/M)
- ρ_d = dry density of the medium, (M/L³)
- n = porosity of the medium, (dimensionless)

Ogata and Banks (1961), solved the advection dispersion equation assuming a constant source concentration, zero initial concentration in the porous media and zero concentration at an infinite distance away from the source. The resulting solution is given as:

$$C_{x,t} = 0.5 \cdot C_0 \cdot \left[\operatorname{erfc} \left(\frac{R \cdot x - v_s \cdot t}{2 \cdot \sqrt{D \cdot t \cdot R}} \right) + \exp \left(\frac{v_s \cdot x}{D} \right) \cdot \operatorname{erfc} \left(\frac{R \cdot x + v_s \cdot t}{2 \cdot \sqrt{D \cdot t \cdot R}} \right) \right] \quad (3)$$

Equation 3 is one of several solutions to the original partial differential ADRE. Details on these equations, their utility and limitations may be found elsewhere (Rabideau and Khandelwal, 1998; Daniels et al., 2000). Software programs such as MYGRT, HYDRUS and MODFLOW/MT3DMS make use of similar equations, often modified for two or three dimensions.

Motivation for this work was provided by the construction of two ash landfills, where it was necessary to evaluate the extent to which leachate could contaminate groundwater. Part of this evaluation involved the characterization of the underlying soils, in terms of their capacity to attenuate trace contaminants. The objective of this paper is to present the observed capacity in terms of batch sorption data, and thereby complement the growing database of physico-chemical interactions in similar systems.

MATERIALS AND METHODS

Batch sorption experiments were conducted in consistence with procedures described by the U.S. Environmental Protection Agency (US EPA 1987). Site soils were mixed and shaken with aqueous concentrations of those constituents determined to be of concern, namely, arsenic (As), barium (Ba), boron (B), cadmium (Cd), chromium (Cr), fluoride (F), lead (Pb), mercury (Hg), nickel (Ni), selenium (Se), silver (Ag) and sulfate (SO₄).

Subsurface drilling and sampling was conducted and representative soil samples were selected at various depths for use in the batch testing conducted herein. Ten samples were selected for each of two sites from various locations and depths as listed in Table 1. Each of the sites was located in the Piedmont region of North Carolina, U.S.A. In general terms, this area is characterized by residual soils. With increasing depth, the soils transition according to three basic layers, typically identified as residuum, saprolite and partially weathered rock (PWR). The concern for groundwater contamination was relegated to the near surface unconfined aquifer, which is frequently in contact with the saprolite and PWR.

Table 1.: Depth of samples collected for Site 1 and Site 2.

Site 1		Site 2	
Sample Number	Approximate Depth Below Ground Surface (m)	Sample Number	Approximate Depth Below Ground Surface (m)
1-1	5	1-2	6
2-1	10	2-2	9
3-1	8	3-2	18
4-1	8	4-2	16
5-1	7	5-2	21
6-1	14	6-2	16
7-1	8	7-2	12
8-1	15	8-2	9
9-1	2	9-2	9
10-1	13	10-2	12

Three soil to solution ratios were investigated with 50 mL polystyrene tubes: 1:5, 1:50 and 1:500. As such, 10 grams, 1 gram and 0.1 grams of material were added to 50 mL of solution, for ratios of 1:5, 1:50 and 1:500, respectively. It is important to either select the correct solid:liquid ratio at the outset or perform iterative testing to establish what ratio is most appropriate. If too little soil is added to a given volume of contaminant solution, then no measurable adsorption will occur and the linear distribution coefficient approaches zero. Likewise, complete adsorption will occur if too much soil is added, reducing the final concentration to zero. In this case, the linear distribution coefficient approaches infinity. In either case, a true indication of sorption capacity cannot be obtained.

From previous experience, the 1:5, 1:50 and 1:500 ratios were selected to generate measurable coefficients for the contaminants of concern. These three ratios were used for all contaminants

except barium and fluoride for which only 1:50 and 1:500 ratios were tested. Again, past experience suggested a measurable K_d could be obtained for these constituents at those two ratios. The required amount of soil was measured using an analytical balance accurate to 0.0001 gram and placed in a labeled container. Samples of the soil were mixed and shaken with aqueous contaminants for a period of 24 hours. Table 2 lists the contaminants and corresponding stock solutions while Table 3 presents the maximum concentration limits allowed in North Carolina (NC), USA, the analytical laboratory reporting limit and the concentration range. With the exception of barium and fluoride, the soils were exposed to the various contaminants simultaneously. For example, the lowest concentration solution is indicated by “Level 1” and consisted of 0.02 mg/L arsenic, 2 mg/L barium and 1 mg/L boron, etc., all mixed together. Barium and fluoride were exposed to the soil specimens in a separate suite of tests to minimize precipitation that is otherwise encouraged when mixed in conjunction with the other contaminants (namely sulfate).

Table 2.: Contaminants of concern, their properties and stock solutions

Constituent	Chemical formula	Potential oxidation state(s)	Stock solution
Arsenic	As	+3, 5	As ₂ O ₃
Barium	Ba	+2	BaCl ₂
Boron	B	+3	H ₃ BO ₃
Cadmium	Cd	+2	Cd(NO ₃) ₂
Chromium	Cr	+6, +3	K ₂ Cr ₂ O ₇
Fluoride	F	-1	CaF ₂
Lead	Pb	+4, +2	Pb(NO ₃) ₂
Mercury	Hg	+2, +1	Hg(NO ₃) ₂ ·H ₂ O
Nickel	Ni	+2, +3	Ni(NO ₃) ₂ ·6H ₂ O
Selenium	Se	+2, +4, +6	SeO ₂
Silver	Ag	+1, +2	AgNO ₃
Sulfate	SO ₄	-2	CaSO ₄

The concentration range is selected on the basis of potential leachate concentration (e.g., from previous leaching tests), analytical detection/reporting limits and the applicable groundwater standard (i.e., the NC regulations). For example, mercury was not observed in previous leaching tests of the sample ash material destined for the landfill. As such, the expected concentration is technically zero. However, it is still desirable to determine a K_d -term in the event there is a change in byproduct type or quality/composition that leads to the presence of mercury. In this case, a concentration range has to be selected without explicit knowledge of potential leachate concentrations. By definition, the next criterion requires that a concentration range that can be measured by the analytical laboratory. Moreover, the concern for soil attenuation generally only arises when the concentration is above the NC 2L groundwater standards. Therefore, the concentration range is selected so that it is above both the analytical/reporting limits of the laboratory and the NC 2L groundwater standards, to some reasonable level.

The metal solutions of varying concentration were added to the soil and the pH was adjusted to 4.44. This pH was selected to simulate precipitation on the basis of historical records for the Piedmont of North Carolina, as discussed in a previous report (Daniels and Das 2006). If the pH

was less, then sodium hydroxide (NaOH) was added to increase the pH and if the pH was greater than 4.44, then nitric acid (HNO₃) was used to reduce the pH. The samples were placed in the shaker for 24 hours at 20⁰C. After 24 hours the samples were centrifuged and the soil was separated from the solution using the vacuum filtration technique. The supernatant was measured for pH and conductivity and then preserved (acidified to pH < 2 and refrigerated at ≈ 4⁰C for metals, refrigerated only for anions) prior to analysis.

Table 3.: Contaminant concentrations used in batch tests.

Contaminant	All Concentrations in mg/L						
	Maximum Concentration Limit as per NC Regulation	Analytical Laboratory Reporting Limit	Target Concentration Range for Batch Tests				
			Level 1	Level 2	Level 3	Level 4	Level 5
Arsenic	0.050	0.0060	0.020	0.040	0.080	0.150	0.300
Barium	2.000	0.0150	2.000	4.000	6.000	8.000	10.000
Boron	0.315	0.3000	1.000	2.000	4.000	6.000	10.000
Cadmium	0.00175	0.0015	0.010	0.025	0.050	0.075	0.150
Chromium	0.050	0.0030	0.050	0.100	0.200	0.500	1.000
Fluoride	2.000	1.0000	2.000	3.000	4.000	5.000	6.000
Lead	0.015	0.0060	0.025	0.050	0.075	0.100	0.150
Mercury	0.00105	0.0004	0.002	0.005	0.010	0.020	0.030
Nickel	0.100	0.0060	0.100	0.200	0.400	0.600	1.000
Selenium	0.050	0.0060	0.050	0.100	0.150	0.200	0.400
Silver	0.0175	0.0015	0.025	0.050	0.075	0.100	0.150
Sulfate	250	5	250	500	750	1000	1500

The analytical results reveal the extent to which the source concentrations (Levels 1-5 in Table 3) decreased in response to shaking with soil. A reduction in metal concentration after the shaking period was attributed to adsorption by or precipitation onto the soil and presented in the form of a linear distribution coefficient. In the event that a measurable K_d-term was generated for more than one solid:liquid ratio, the ratio which corresponded to approximately 10 to 30% adsorption was selected. If more than one solid:liquid ratio resulted in adsorption in this range, then the values were averaged. The 10 to 30% range of adsorption is recommended to maximize data quality and repeatability (US EPA 1987). All batch tests were done in triplicate, i.e., three samples for each metal solution and solid sample. The resulting supernatant from each of the three tests was then combined to make one aqueous sample for subsequent analytical testing. The amount adsorbed per mass of adsorbent was calculated as follows:

$$\frac{x}{m} = \frac{(C_o - C)}{m} V \quad (4)$$

Where x/m is the solid phase concentration (mg/g), C_o is the initial concentration (mg/L), C is the final concentration (mg/L), m is the mass of material used (g) and V is the volume of solution (L). The K_d-term is taken as the slope of the solid phase concentration (x/m) versus the final aqueous concentration (C), and the units are frequently reported in mL/g.

All glassware and sampling tubes were flushed with tap water, secondly flushed with a detergent (citronox) then with de-ionized water, acid washed with 10% HNO₃ and finally rinsed with de-ionized water. A stock solution of 1000 mg/L was used where 5 mL was pipetted into a 50 mL volumetric flask and the volume was raised to 50 mL using de-ionized water. In the case of fluoride and sulfate, their respective (CaF₂ and CaSO₄) salts were used. This results in a concentration of 100 mg/l. The remaining concentrations were prepared using this solution. Once the solutions were prepared, the pH was adjusted to 4.44 as noted above.

RESULTS AND DISCUSSION

The results of the pH measurements for Site 1 and Site 2 are provided in Tables 4-6 and Tables 7-9, respectively. These results are given primarily for information purposes only, i.e., they are not used in the calculation of the distribution coefficient (K_d -term). However, the distribution coefficient is sensitive to solution conditions, including pH, conductivity and temperature. As noted above, the initial pH of the solutions was 4.44 and the temperature was maintained at 20°C throughout the test. During the course of the batch sorption test, the pH and conductivity change as the soil is shaken with the contaminant solution. Most of the pH and conductivity readings (conductivity data not included herein) appear to reasonably reflect the nature of the batch sorption test.

Table 4.: Final pH values for 1:5 Ratio – Site 1.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44)				
	1:5 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-1	4.75	4.39	4.26	3.65	3.49
2-1	4.40	3.78	3.82	3.66	3.29
3-1	4.12	3.99	3.87	3.74	3.46
4-1	4.40	4.27	4.26	4.14	4.14
5-1	4.53	4.55	4.57	4.30	4.21
6-1	5.74	5.52	5.10	4.76	4.35
7-1	5.92	5.56	5.04	4.75	4.51
8-1	3.86	5.31	5.25	4.91	4.63
9-1	5.45	5.15	4.88	4.50	4.11
10-1	4.81	4.85	4.74	4.61	3.92

Table 5.: Final pH values for 1:50 Ratio – Site 1.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44)				
	1:50 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-1	4.63	4.12	3.88	3.62	3.41
2-1	4.32	4.24	4.00	3.69	3.30
3-1	4.63	4.54	4.79	3.95	3.43
4-1	4.33	4.10	3.99	3.77	3.40
5-1	4.69	4.25	3.92	3.70	3.75

6-1	4.48	3.75	3.48	3.09	2.99
7-1	4.51	3.91	3.49	3.19	2.90
8-1	4.68	3.93	3.61	3.38	3.26
9-1	4.18	3.66	3.33	3.21	3.16
10-1	4.77	4.37	3.83	3.83	3.10

Table 6.: Final pH values for 1:500 Ratio – Site 1.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44) 1:500 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-1	5.34	4.93	3.7	4.4	4.25
2-1	5.47	4.74	4.62	4.67	5.13
3-1	4.03	4	3.86	3.54	3.86
4-1	3.87	3.48	3.34	2.85	2.79
5-1	3.92	3.56	2.42	3.01	2.94
6-1	4.74	4.43	4.18	3.87	3.75
7-1	4.67	4.38	4.16	3.94	3.61
8-1	4.61	4.46	4.31	4.09	4.01
9-1	4.93	4.46	4.12	4.03	3.81
10-1	4.78	4.44	4.17	4.01	3.91

Table 7.: Final pH values for 1:5 Ratio – Site 2.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44) 1:5 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-2	5.09	4.99	4.90	4.65	4.46
2-2	4.28	4.10	4.04	3.94	4.27
3-2	5.52	5.39	5.67	4.98	4.62
4-2	5.43	5.40	5.22	5.10	4.86
5-2	5.77	5.65	5.63	5.25	5.22
6-2	5.12	4.82	4.79	4.63	4.55
7-2	5.59	5.68	5.67	5.56	5.48
8-2	5.29	5.29	4.97	4.64	4.50
9-2	5.39	5.24	5.27	5.08	5.01
10-2	5.44	5.51	5.62	5.45	5.21

Table 8.: Final pH values for 1:50 Ratio – Site 2.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44) 1:50 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-2	4.77	4.41	3.73	3.07	2.85
2-2	4.52	3.63	3.55	3.94	3.61
3-2	5.09	4.51	4.03	3.51	3.28
4-2	4.53	4.50	3.93	3.31	2.39
5-2	4.66	4.70	4.56	3.16	2.93

6-2	3.92	3.82	3.44	4.13	2.54
7-2	4.84	4.63	4.27	3.69	3.42
8-2	4.60	4.25	3.88	3.15	2.88
9-2	4.48	4.30	4.08	3.57	3.51
10-2	4.30	4.04	3.47	2.97	2.51

Table 9.: Final pH values for 1:500 Ratio – Site 2.

Sample Number	pH Value after Batch Sorption Test (initial pH = 4.44) 1:500 Ratio				
	Level 1	Level 2	Level 3	Level 4	Level 5
1-2	5.08	4.85	4.64	4.11	3.76
2-2	5.21	5.01	4.34	4.34	3.58
3-2	4.71	4.27	4.10	3.91	3.43
4-2	5.06	4.52	4.23	3.92	3.93
5-2	5.77	4.80	4.30	4.99	3.88
6-2	5.26	4.47	4.30	4.47	4.47
7-2	5.13	4.71	4.43	4.74	3.70
8-2	5.26	4.83	4.41	3.96	3.87
9-2	4.17	4.94	4.41	4.35	4.30
10-2	4.75	4.04	4.00	3.96	3.51

In addition to measuring the supernatant concentrations, the target source concentrations (presented previously as Table 3.) were also measured. The purpose of this step was to verify the extent to which the desired source concentrations were achieved. While the target concentrations are prepared with known solutions as discussed in the Materials and Methods section, variability is expected, for several reasons. First, laboratory-grade stock solutions are typically provided to an accuracy of about ± 1 mg/L. Subsequent dilutions for preparation of the target concentrations naturally propagate this potential error. Secondly, while each of the contaminants is added to the overall solution in a known amount, the extent to which they remain in solution is dictated by their relative interaction with other constituents. The measured concentrations are presented in Table 10, although it should be noted that these concentrations are for one sample of the source concentration. The source concentration was prepared in many different batches over different days and there is likely to be variability therein.

Table 10.: Measured concentrations in source solutions.

Contaminant	All Concentrations in mg/L						
	NC 2L Standard	Analytical Laboratory Reporting Limit	Measured Concentration Range for Batch Tests				
			Level 1	Level 2	Level 3	Level 4	Level 5
Arsenic	0.050	0.0060	0.02681	0.05342	0.108	0.1892	0.3696
Barium	2.000	0.0150	1.804	3.779	5.757	7.716	9.673
Boron	0.315	0.3000	1.017	1.93	3.8	5.61	9.429
Cadmium	0.00175	0.0015	0.01159	0.02799	0.05653	0.08419	0.1613
Chromium	0.050	0.0030	0.05551	0.1096	0.2193	0.5318	1.031
Fluoride	2.000	1.0000	1.9	1.4	1.6	1.6	2.6

Lead	0.015	0.0060	0.02773	0.05491	0.08366	0.1128	0.1676
Mercury	0.00105	0.0004	0.0011	0.004	0.0077	0.020	0.030
Nickel	0.100	0.0060	0.1062	0.209	0.414	0.6122	0.9658
Selenium	0.050	0.0060	0.06948	0.132	0.1965	0.2553	0.5065
Silver	0.0175	0.0015	0.02573	0.05071	0.07811	0.1013	0.1499
Sulfate	250	5	173.86	387.8	497.96	775.96	1150

The final distribution coefficients (K_d values) are given in Table 11 and 12 for Site 1 and Site 2, respectively. It is the values in these final tables that may be used in groundwater modeling applications to simulate attenuation of the contaminants investigated, namely, arsenic, barium, boron, cadmium, chromium, fluoride, lead, mercury, nickel, selenium, silver and sulfate. As noted in Tables 11 and 12, there is considerable scatter in the data obtained. Moreover, there were some soil/contaminant combinations for which an explicit K_d could not be calculated. For example, in the case of fluoride for Site 1 and lead for Site 2, the final concentrations at even the lowest soil:solution ratio were close to the detection limits. These values were thus estimated in terms of the likely range.

Given the limitations associated with linear distribution coefficients, one might question if there is any value at all in their measurement or use. Difficulties with this approach have been observed with respect to nuclear waste containment, e.g., radionuclides (Moody 1982). In addition, Domenico and Schwartz (1998), note that a K_d approach is too simplistic to accurately model the complicated nature of metal-soil interaction. The authors suggest a more rigorous approach that accounts for the dynamic properties of both the solution and the sorbent is necessary. Indeed, there are several factors that are likely to result in a difference between actual contaminant transport and that predicted on the basis of models using the K_d approach, as summarized in Table 13. Many alternative models have been developed as summarized by Turner and Fein (2007), who observe that better agreement has been found through application of a physically-based dual porosity model or a chemically-based rate-limited sorption approach. The former method presumes that a mobile fraction of the pore space is available for advection/dispersion processes. Overall contaminant transport is then a function of the extent to which this fraction interacts with an immobile portion that is defined in terms of diffusion. Similarly, the rate-limited approach applies some a priori assumption on the kinetics (often first order or pseudo-first order) at which a given contaminant will interact with the surrounding media.

Clearly, the K_d approach has substantial limitations for accurate modeling of contaminant transport. However, K_d measurements can easily be made over a range of solution (pH, Eh, conductivity, etc.) conditions to better reflect in situ conditions. Likewise, there remain many circumstances for which local equilibrium is established, the reaction is reversible and the isotherm is linear (Freeze and Cherry 1979). Work conducted by Bin-Shafique et al. (2002) to evaluate transport of trace metals made successful use of a K_d -based approach to match numerical, laboratory and field data. Moreover, values of K_d need not be precise to be of value, particularly when noted to be rather large. In particular, Freeze and Cherry (1979) also note that K_d values that are orders of magnitude larger than unity are considered “immobile”. Finally, because they are simple to obtain and to employ, the use of K_d values is likely to continue.

Table 11.: Final distribution coefficients (K_d values) for Site 1.

Sample Number	K_d values, mL/g											
	As	Ba	B	Cd	Cr	F	Hg	Pb	Ni	Se	Ag	SO ₄
1-1	91.88	27.73	1.11	4.14	47.84	500.00	49.30	56.40	5.06	94.73	51.57	6.26
2-1	130.46	49.81	~0	2.53	33.24	500.00	212.38	112.80	3.70	149.29	66.69	6.57
3-1	142.26	20.09	3.75	0.42	5.87	308.33	110.80	58.60	5.64	147.68	8.42	6.34
4-1	176.19	40.64	~0	2.75	16.11	64.29	79.61	77.58	7.66	211.78	16.18	6.18
5-1	222.34	75.68	0.30	7.54	5.13	375.00	172.25	126.92	20.84	274.58	10.97	5.56
6-1	113.54	47.52	0.004	11.26	1.85	166.67	295.81	106.59	3.08	135.48	22.84	22.55
7-1	59.75	84.06	0.10	9.48	0.88	500.00	285.97	105.95	0.49	68.56	32.70	1.97
8-1	93.95	107.84	0.15	10.01	0.81	-	134.69	86.84	0.88	103.04	29.09	1.92
9-1	55.61	14.32	0.11	0.72	0.74	> 100	107.22	43.53	0.23	30.13	80.01	1.52
10-1	24.90	5.40	0.10	0.64	0.81	1166.67	159.69	35.81	0.29	15.27	5.59	2.23

Table 12. Final distribution coefficients (K_d values) for Site 2.

Sample Number	K_d values, mL/g											
	As	Ba	B	Cd	Cr	F	Hg	Pb	Ni	Se	Ag	SO ₄
1-2	92.07	631.70	0.24	1.36	7.81	102.53	4.34	> 2590	12.35	168.16	149.94	12.47
2-2	285.59	459.57	4.98	52.45	4.56	101.09	46.63	> 1000	5.08	172.22	222.49	11.41
3-2	53.70	532.93	0.33	1.53	0.80	107.38	20.85	> 2350	2.40	227.83	51.00	4.80
4-2	106.28	439.32	0.19	6.23	28.51	62.92	21.99	> 2580	14.02	406.24	128.18	0.94
5-2	372.30	457.98	0.23	0.98	1.03	117.91	4.97	> 1000	0.62	172.94	182.30	4.00
6-2	121.48	367.05	0.53	1.53	14.58	87.76	20.67	> 2150	14.09	220.67	29.37	3.05
7-2	125.49	94.49	0.22	2.14	13.15	74.87	67.49	> 1000	19.72	189.06	56.22	1.10
8-2	61.99	182.19	0.48	1.80	1.71	117.89	40.28	> 1000	1.66	53.25	103.58	2.17
9-2	125.19	533.46	0.48	1.27	0.86	16.72	110.88	> 1760	0.79	128.40	88.71	1.81
10-2	493.98	52.26	0.24	0.84	18.34	219.11	27.62	> 2800	34.44	260.06	31.07	4.00

Table 13.: Example limitations of a linear distribution coefficient (K_d) approach to contaminant transport modeling (not exhaustive).

K_d Approach Assumptions / Characteristics	Potential Limitations In Situ
Linearity between liquid and solid phase contaminant concentration	Non-linear relationship
Local equilibrium between liquid and solid phase contaminant concentration	Existence of non-equilibrium conditions
Reversible reaction mechanism	Irreversible reactions
Low solid:liquid ratio (often < 1:10)	High solid:liquid ratio (> 1:1)
Laboratory controlled pore fluid conditions in terms of pH, Eh, conductivity, etc.	Temporal and spatial variability in pore fluid conditions, presence of bacteria, etc.

CONCLUSIONS

While limited to the conditions under which they are generated, batch sorption data may be used to approximate the capacity of soils to attenuate various contaminants. Twenty soil samples across two different sites were tested for such capacity with respect to twelve different contaminants. For Site 1, boron shows the least adsorption ($0 \text{ mL/g} < K_d < 3.75 \text{ mL/g}$) while fluoride shows the highest ($64 \text{ mL/g} < K_d < 1167 \text{ mL/g}$). Similarly, for Site 2, boron also shows the least adsorption ($0.19 \text{ mL/g} < K_d < 4.98 \text{ mL/g}$) while lead shows the highest ($K_d > 1000 \text{ mL/g}$).

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