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Memorandum

Date: February 26, 2003

To: John Pietz

From: Jonathan Myers

RE: Sorption Coefficients for RDX and Barium at Los Alamos

This memo provides the results of a literature review of RDX and barium sorption coefficients for use at Los Alamos.

RDX Sorption

RDX has a strong affinity for sorption on organic carbon, which is why the standard treatment process for contaminated waste water is sorption on granular activated carbon. Some organic carbon partition coefficients (K_{oc}) cited in the literature are as follows:

Koc (mL/g)	Reference	
100	Rosenblatt, 1986	
135	Tucker et al., 1985	
7.8 to 269	Sikka et al.,1980	
42 to 126	Spanggord et al., 1980	

The affinity for sorption of RDX on low-carbon soils, sediment, and specific soil-forming minerals is considerably less than that of organic carbon. The sorption of RDX on soils has been studied by several researchers (Sikka et al. 1980; Leggett 1985; Ainsworth et al. 1993; Selim and Iskandar 1994; Townsend and Myers, 1996). Each of these researchers found that RDX was extremely mobile and could be described well using a linear equilibrium approach. Leggett (1985) noted that sorption values for RDX on bentonite drilling muds were similar to sorption values for RDX on natural sediments, suggesting that the clay content of natural soils and sediments is important to the sorption of RDX. Reported linear equilibrium distribution coefficients for RDX on natural soils and sediments range from <1 to 7.8 mL/g (Townsend and Myers 1996).

Ainsworth et al. (1993) performed batch and column tests with RDX. In both the batch and column tests, RDX sorption fit a linear model, and was found to be reversible.



Townsend et al. (1996) performed column flow-through sorption experiments on three soils: Tunica silt from Vicksburg, MS, Yokem clay from Vicksburg, MS, and Ottawa sand obtained from U.S. Silica Company, Ottawa, IL. Linear equilibrium distribution coefficients (K_d) for RDX were 2.5, 5.7, and 1.35 mL/g for the Tunica silt, Yokena clay, and Ottawa sand, respectively, and scale with increasing clay content. These coefficients are in good agreement with those reported in previous works (Townsend and Myers 1996, McGrath 1995).

Zakikhani et al., 2002 evaluated the sorption of explosives including RDX at the Louisiana Army Ammunition Plant (LAAP). Aquifer soils from LAAP were generally high in sand, ranging from 65.0 to 92.5 percent sand. Silt and clay were present in all samples in lower amounts. Total organic carbon content was low, ranging from 0.015 to 0.162 percent. Cation exchange capacity (CEC) was also low, ranging from 3.5 to 8.1 Meq 100 g⁻¹. Soil pH was acidic and relatively consistent for all soil types (average of 5.55). Permeabilities of the soils ranged from 10^{-4} to 10^{-9} cm sec⁻¹.

Adsorption of explosives from groundwater by the LAAP aquifer soils was limited. The measured values of K_d were below 1mL/ g for all soils and contaminants, ranging from no significant adsorption to a high value of 0.84 mL/g. The highest degree of sorption was associated with the soils highest in clay and CEC. They concluded that mass transport limitations other than sorption (such as low permeability) are limiting factors for transport of HE at LAAP.

K _d (mL/g)	Reference	
0.2 to 7.8	Hale, et al., 1979	
0.8 to 4.15	Sikka et al.,1980	
1.4 to 4.2	Spanggord et al., 1980	
4.92 to6.75	Leggett, 1985	
<1	Ainsworth et al., 1993	
0.0 to 0.8	Myers et al. (in preparation)	

Some additional experimentally determined K_d values for RDX are as follows:

Barium Sorption

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Barium has an affinity for adsorption on clays, oxides, and hydrous oxides in soil. The relative affinity of alkaline earth cations for cation exchange and specific adsorption sites on clays and oxides decreases in the order Ba > Sr > Ca > Mg (EPRI, 1984). Barium would thus be expected to displace Ca and Mg from sorption sites. Surface complexation by soil organic matter also occurs to a limited extent. Adsorption coefficients for barium are provided in the following table.

	Adsorption Coefficients (mL/g)	Substrate	Source	Range (mL/g)
Barium	$K_d = 66$	Unweathered glacial till	IT, 1993	K _d = 66 to 2,800
	K _d = 128	Weathered glacial till	IT, 1993	
	K _d = 2,800	Sediment/ River water	Li and Chan, 1979	

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