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CONSULTING ENGINEERS, INC.

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Volume 2-Appendices

Report 3 Environmental Effects of Present & Proposed Tailings Disposal Practices

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APPENDIX J
SENSITIVITY ANALYSIS OF DISPERSION PARAMETERS

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APPENDIX J

SENSITIVITY ANALYSIS OF DISPERSION PARAMETERS

The degree of spreading and mobility (dispersion) of any substance in a porous media depends on the behavior of that specific substance and the environment in which the dispersion is taking place. Factors that control dispersion phenomena are defined by parameters most of which are empirical. These parameters can be grouped into three categories:

- Substance dependent such as decay constant
- Media dependent such as intrinsic permeability
- Substance-environment dependent such as distribution coefficient

Most mass transport parameters are directly or indirectly in the third category. For example fluid velocity is affected by the concentration gradient and consequently, effects the dispersion; or the solution pH changes the distribution coefficient. Important parameters which contribute to the migration of a substance are as follows:

- Pore velocity (function of hydraulic gradient, permeability, effective porosity)
- Dispersion coefficient (function of velocity, dispersivity)
- Equilibrium constant (function of distribution coefficient, unit weight and porosity of the porous media)
- Decay constant

The sensitivity of these parameters (except decay constant) to the rate of migration of a substance is analyzed by the dimensionless solution of one dimensional dispersion.

The equation for a one dimensional ion exchange column is as follows (Lapidus and Amundson [Duguid and Reeves, 1976]):

$$R_d \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial z} \quad (1)$$

where

D = Longitudinal dispersion coefficient [L^2/t]

V = Pore velocity = $-K\Delta h/n_e$ [L/t]

K = Permeability [L/t]

Δh = Piezometric head difference [L]

n_e = Effective porosity

C = Concentration of a chemical species [M/L^3]

R_d = Adsorption equilibrium constant or retardation factor [nondimensional]

t = Time [t]

$\frac{\partial}{\partial z}$, $\frac{\partial}{\partial t}$ = Partial derivatives with respect to z and t .

Equation (1) can be written as

$$\frac{\partial C}{\partial t} = \overset{*}{D} \frac{\partial^2 C}{\partial z^2} - \overset{*}{V} \frac{\partial C}{\partial z} \quad (2)$$

where

$$\overset{*}{D} = D/R_d \text{ and } \overset{*}{V} = V/R_d$$

With the following initial and boundary conditions

$$C(0,t) = C_0; t \geq 0$$

$$C(z,0) = 0; z \geq 0$$

$$C(\infty,t) = 0; t \geq 0$$

The solution of Equation (1) yields

$$\frac{C}{C_0} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{z - \overset{*}{V}t}{2\sqrt{\overset{*}{D}t}} \right) + \exp \left(\frac{\overset{*}{V}z}{\overset{*}{D}} \right) \operatorname{erfc} \left(\frac{z + \overset{*}{V}t}{2\sqrt{\overset{*}{D}t}} \right) \right] \quad (4)$$

The dimensionless parameters ξ , η are defined as

$$\xi = \frac{Vt^*}{z} = \frac{Vt}{R_d z} = \frac{V}{z} t^* \quad [t^* \text{ retarded time due to adsorption process}] \quad (5)$$

$$\eta = \frac{D}{Vz} = \frac{D}{Vz} \quad (6)$$

Substituting ξ , η into Equation (4) yields

$$\frac{C}{C_0} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{1 - \xi}{2\sqrt{\xi\eta}} \right) + \exp(1/\eta) \operatorname{erfc} \left(\frac{1 + \xi}{2\sqrt{\xi\eta}} \right) \right] \quad (7)$$

Equation (7) is used to obtain the dimensionless concentration with respect to different ξ and η values. The calculated concentrations are plotted versus ξ on a semilog paper for different η values as shown in Figure J-2. Two major observations made from this figure are:

1. The shape of the concentration curve is independent of ξ and is a function of η only. Where η decreases, the slope of the curve (measured at $C/C_0 = 0.5$) increases. As η approaches zero, the slope of the curve approaches 90 degrees. Another observation is that the larger η value covers more ranges of ξ .
2. Regardless of the η value (except for $\eta > 0.02$) at ξ equal to one, the dimensionless concentration is 0.5.

The specific conclusions made from above observations are as follows:

1. The dissolved substance will spread more at a larger η than smaller one. For example, at $\xi = 0.7$, the concentration is 0.06 and 0.16 for η equal to

0.025 and 0.05, respectively. But as η decreases the concentration difference of two curve also decreases. This implies at very small η , say less than 0.01, the concentration curve will not substantially change. In other words, the shape of the spreading becomes independent of η when η is less than 0.01.

Accepting the linear relationship between dispersion coefficient and velocity vectors, i.e., $D_I = a_I V$, the dimensionless η value can be written as:

$$\eta = a_I / z$$

This equation states that η is a function of longitudinal dispersivity and distance and almost independent of velocity. It can be concluded that shape of spreading is controlled strongly by longitudinal dispersivity and distance from the source. It is also noted that the concentration is 0.5 at $\xi = 1$ regardless of the value η .

2. Figure J-2 shows that generally the change of concentration starts at ξ greater than 0.1 and beyond $\xi = 2$ the concentration almost attains its source value. To assure a contaminant will not reach a point, the value of ξ should be less than 0.1. Examination of parameters which constitute ξ , reveals that velocity and time increase ξ , while the equilibrium constant and distance decrease its value. This implies that those four parameters have identical effect in migration or mitigation of any substances (e.g., radionuclide).

The following conclusions are derived from the above discussions:

- a. For nonadsorbing dissolved tracers (materials present in very low dissolved concentrations), such as sulfate, or fluoride, where $R_d = 1$, the major controlling factor is the hydrogeological parameter, i.e., movement of material can be retarded by reducing velocity.
- b. For all adsorbing substances velocity vectors and equilibrium constants are major factors. Typical values of distribution coefficients and equilibrium constants at different pH values for a few radionuclides are given in Table J-1. The equilibrium constant for each element is different and increases with increasing pH. To control migration of radionuclides not only the flow regime should be controlled, but it is more important that the pH of the water be maintained in the higher pH required, e.g. pH = 6 or above.

APPENDIX J
REFERENCE

1. Duguid, J. O. and M. Reeves, 1976, "Material Transport Through Porous Media: A Finite Element Galerkin Model," Environmental Sciences Division Publication 733, Oak Ridge National Laboratory, National Technical Information Service, Springfield, Virginia, 201 pp.

TABLE J.1
 DISTRIBUTION COEFFICIENTS AND DECAY CONSTANTS
 USED IN COMPUTER MODELING OF CHEMICAL DISPERSION

ELEMENT	pH	DISTRIBUTION COEFFICIENT K_d (ml/g)	ADSORPTION EQUILIBRIUM CONSTANT R_d	DECAY CONSTANT ⁽¹⁾ λ (month ⁻¹)
As	2.0	0 ⁽²⁾	1	Stable
	4.5	25 ⁽²⁾	95	
	5.75	200 ⁽³⁾	755	
	7.0	300 ⁽²⁾	1,135	
U-238 ⁽⁵⁾	2.0	100 ⁽²⁾	380	1.3×10^{-11}
	4.5	200 ⁽²⁾	755	
	5.75	1,000 ⁽³⁾	3,780	
	7.0	2,000 ⁽²⁾	7,560	
Th-230	2.0	16 ⁽²⁾	60	7.2×10^{-7}
	4.5	5,000 ⁽³⁾	18,900	
	5.75	10,000 ⁽³⁾	37,800	
	7.0	15,000 ⁽⁴⁾	56,710	
Ra-226	2.0	0 ⁽²⁾	1	3.6×10^{-5}
	4.5	12 ⁽³⁾	45	
	5.75	60 ⁽³⁾	225	
	7.0	100 ⁽⁴⁾	380	
Pb-210 ⁽⁵⁾	2.0	20 ⁽²⁾	75	2.8×10^{-3}
	4.5	100 ⁽²⁾	380	
	5.75	1,500 ⁽³⁾	5,670	
	7.0	4,000 ⁽²⁾	15,120	
Po-210	2.0	0 ⁽³⁾	1	1.5×10^{-1}
	4.5	0 ⁽³⁾	1	
	5.75	12 ⁽³⁾	45	
	7.0	25 ⁽⁴⁾	95	

NOTES:

- (1) From Lederer, et al., 1967.
- (2) Determined for site sediments.
- (3) Estimated.
- (4) Estimated from literature.
- (5) Determination made from total uranium and lead assumed equal to K_d of U-238 or Pb-210.

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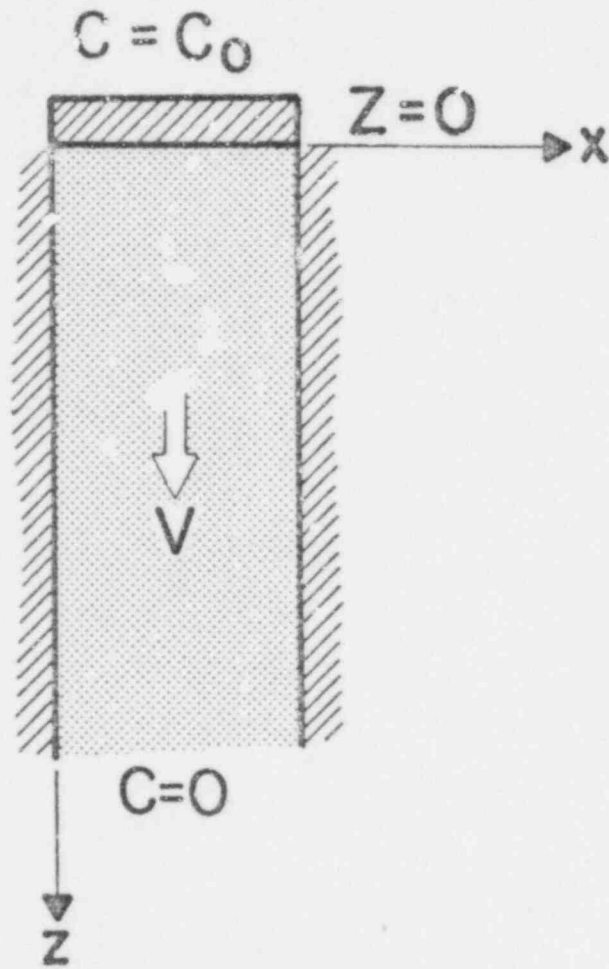


FIGURE J-1
SCHEMATIC DIAGRAM OF
ONE DIMENSIONAL
LONGITUDINAL DISPERSION

PREPARED FOR

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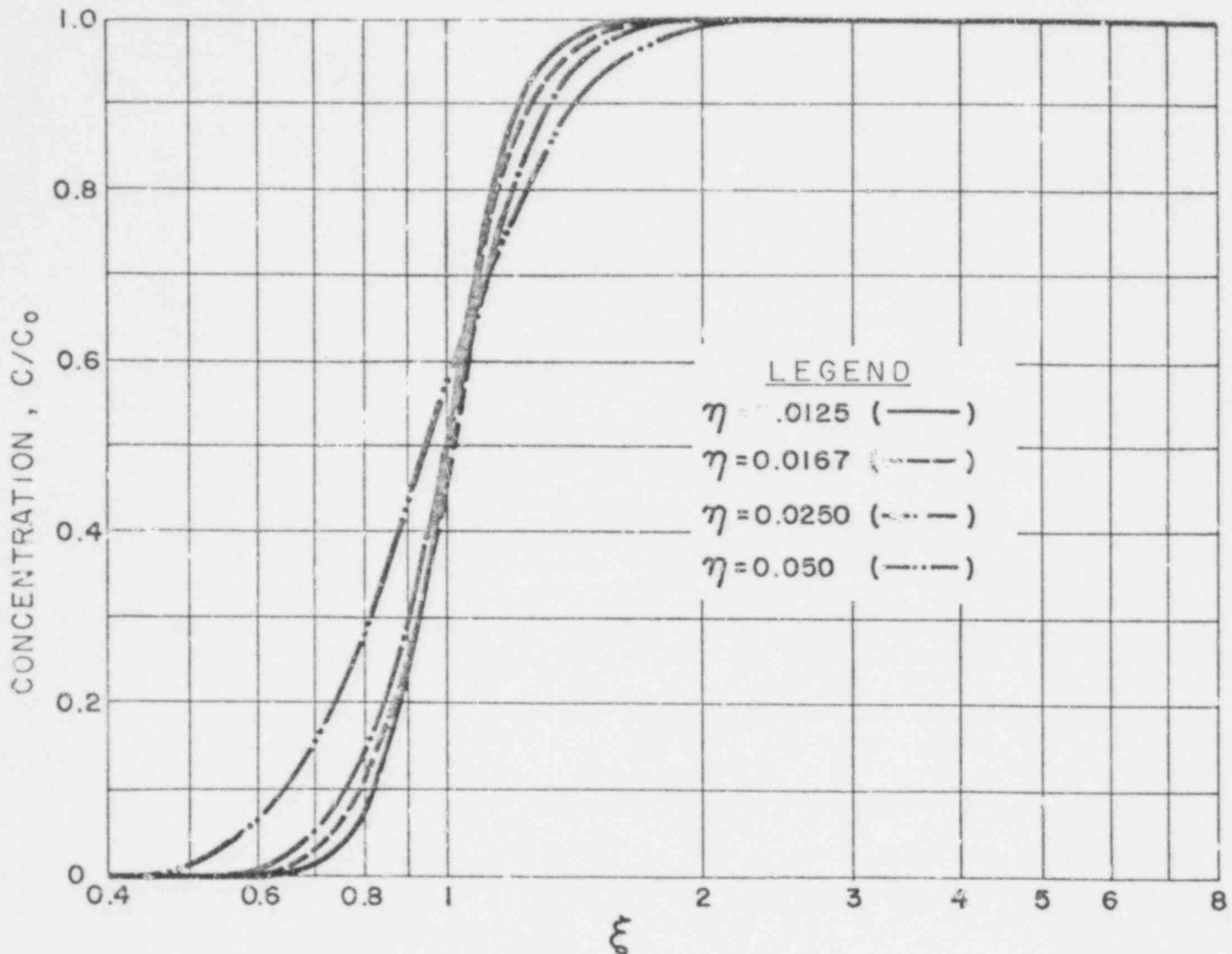


FIGURE J-2
CONCENTRATION DISTRIBUTION
VERSUS ξ
FOR DIFFERENT VALUES OF η

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