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Comparison of Contaminant Transport between the Centrifuge Model and the Advection Dispersion Equation Model

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ABSTRACT

The centrifuge test result on capped sediment was compared to the advection- dispersion equation proposed for one layered to predict contaminant transport parameters. The fitted contaminant transport parameters for the centrifuge test results were one to three orders of magnitude greater than the estimated parameters from the advection-dispersion equation. This indicates that the centrifuge model over estimated the contaminant transport phenomena. Thus, the centrifuge provides a non-conservative approach to modeling contaminant transport. It should be also noted that the advection-dispersion equation used in this study is a one layered model. Two layered modeling approaches are more appropriate for modeling this data since there are two layers with different partitioning coefficients. Further research is required to model the centrifuge test using two-layered advection-dispersion models.

Keywords : advection-dispersion equation, one layered model, contaminant transport, centrifuge

1. Introduction

Laboratory procedures are available for estimating contaminant migration from sediment into caps by diffusion[2,6,9,11]), but diffusion may not be the major process affecting capping effectiveness. Thibodeaux *et al.* (1998) developed the vignette chemodynamic model to estimate the advected pore water into the cap. Thibodeaux *et al.* modeling approach showed that the PCB that emerged from the contaminated sediment were immobilized onto the solid surfaces after moving only a short distance into the cap material. Movement of contaminated pore water from sediment into caps due to sediment consolidation during and after cap placement may be much more significant than contaminant diffusion into caps. However, there is a basic lack of information on the significance of consolidation induced advective transport of contaminants from contaminated sediment into caps.

Thus, centrifuge test was conducted to monitor the consolidation induced advective transport using a carbon-14 radio-labeled compound, 2,3,7,8-tetrachloro[U-14]dibenzo-p-dioxin ([^{14}C]TCDD) (referred to as TCDD throughout the rest of the document) purchased from Chemsyn Science Laboratories[4]). TCDD was used in order to quantify the dioxin concentrations in thin sections of sediment and cap materials and in small quantities of water. TCDD is a beta emitter that has a half-life of 5730 years and emits 0.156 MeV. Calculations were based on the minimum carbon-14 activity required to obtain reproducible liquid scintillation counts on a 200-micron slice. The New York Dredged Material Management Plan (NYDMMP) sediment was spiked at a concentration of 24 μg/kg of TCDD. TCDD was measured using a liquid scintillation counter. Because of safety concerns involved, tests were conducted as a semi-sealed source test with no instrumentation for measuring sediment settlement. Figure 1 shows the TCDD concentration (in μg/l) versus the prototype time for the overlying water samples obtained during the centrifuge tests and shows that the maximum concentration of TCDD advected from the sediment was 0.024 μg/l. Centrifuge test results clearly illustrated that advection and dispersion are dominated the migration of contaminants[4]).

In this paper, the advection dispersion equation proposed for one layer was described and the centrifuge test result was compared to this equation used to estimate transport parameters of the centrifuge model. Sensitivity analysis was also conducted on the advection dispersion equation and suggested further researches that are needed to improve the modeling on the contaminant transport through capped dredged sediment.

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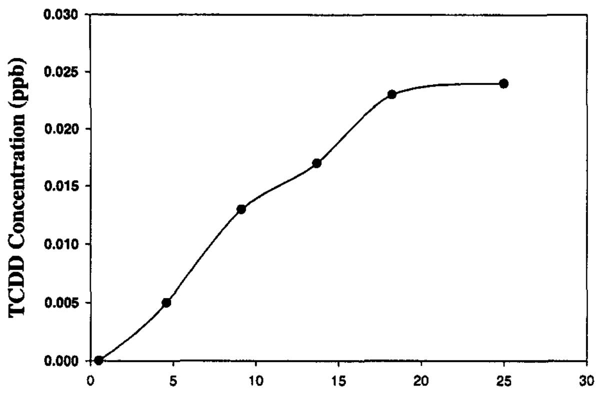

Fig. 1. TCDD concentration in overlying water in centrifuge test II (From Moo-Young and Kim, 2003).

2. Modeling utilizing the advection dispersion equation

Advection, hydrodynamic dispersion, and sorption govern the transport of contaminants through porous media[3]. Van Genuchten and Alves (1982) have provided a compendium of many analytical solutions to the advection dispersion equation. The one-dimensional form of the advection-dispersion equation with linear equilibrium-controlled sorption and no reaction is as follows:

$$R_f\frac{\partial c}{\partial t}=D_A\frac{\partial^2 c}{\partial z^2}-v_z\frac{\partial c}{\partial z} \tag{1}$$

where t = Time
v_z = seepage velocity
z = depth
R_f = retardation factor = $1 + K_d\,\rho/n$
D_A = hydrodynamic dispersion coefficient
c = concentration
n = porosity
ρ = density
K_d = Partitioning coefficient = S/C, l/kg (2)

where S = contaminant concentration in the sediment at equilibrium, mg/kg
C = Contaminant concentration in the aqueous phase at equilibrium, mg/l

In this portion of the study, advection dispersion equation was used to estimate transport parameters of the centrifuge model. Moreover, in studying the transport of TCDD through the cap, the semi-infinite region with uniform initial concentration with a constant flux boundary condition model was utilized. The initial and boundary conditions were as follows:

$$c(z,t)|_{t=0}=c_i \qquad z\in[0,0]$$

$$-D_A\frac{\partial c}{\partial z}|_{z=0}+v_z\cdot c(z,t)|_{z=0}=v_z\cdot c_o \qquad t>0 \tag{3}$$

$$\frac{\partial c}{\partial z}|_{z\to\infty}=0 \tag{4}$$

The solution with the initial and boundary conditions given above is as follows:

$$c(z,t)=c_i+(c_o-c_i)\left[\begin{array}{l}\frac{1}{2}erfc\left(\frac{R_fz-v_zt}{2\sqrt{D_AR_ft}}\right)+\sqrt{\frac{v_z^2t}{\pi D_AR_f}}\exp-\frac{(R_fz-v_zt)^2}{4D_AR_ft}\\ -\frac{1}{2}\left(1+\frac{v_zz}{D_A}+\frac{v_z^2t}{D_AR_f}\right)\exp\pm\left(\frac{v_zz}{D_A}\right)erfc\left(\frac{R_fz+v_zt}{2\sqrt{D_AR_ft}}\right)\end{array}\right] \tag{5}$$

3. Sensitivity analysis

Prior to conducting the sensitivity analysis, reasonable estimates of the transport parameters in Eq. 5 were made. Table 1 shows the properties of TCDD, sediment, capping material, and contamination parameters used in the model. For the sediment and capping materials, the partitioning coefficient was estimated by the following equations

$$K_d = K_{oc}f_{oc} \tag{6}$$

Table 1. Contaminant Transport Modeling Parameters for Capping Material

TCDD	Properties
Molecular weight	321.9
Diffusion coefficient in water (cm^2/s)	5.6×10^{-6}
Aqueous solubility (mg/l)	0.0002
Octanol-water partitioning coefficient, log K_{ow}	6.72
Organic carbon partitioning coefficient, log K_{oc}	6.51
Sediment	
Bulk density (g/cm^3)	0.3
Organic carbon fraction	0.026
Depth (cm)	900
Porosity	0.75
Water content (%)	110
Estimated partitioning coefficient, (cm^3/g)	84134
Contaminant concentration in sediment (μg/Kg)	24
Estimated contaminant concentration in aqueous phase (μg/l)	0.031
Cap	
Bulk density (g/cm^3)	1.6
Organic carbon fraction	0.002
Effective capping depth (cm)	0-300
Porosity	0.44
Water content	0.3
Estimated partitioning coefficient (cm^3/g)	6471
Estimated velocity (cm/sec)	1×10^{-3}
Estimated hydrodynamic dispersion (cm^2/sec)	1×10^{-5}

Table 2. Physical Characteristics of Sediment and Cap (From Moo-Young and Kim, 2003)

Parameter	ASTM method	Sediment	Cap
% Sand	D-422	33	94
% Fines	D-422	66	6
Water content (%)	D-2216	113	29
Organic content (%)	D-2974	2.6	0.2
Density g/cm^3 (pcf)	--	1.4 (88)	1.95 (121)
Specific gravity	D-845	2.64	2.68
Void ratio	--	2.98	0.77
Porosity	--	0.75	0.44
Soil classification	D-2487	CH	SP-SM
Effective size, D_{10} (mm)		0.004	0.17
Mean particle diameter (mm)		.06	0.35
Hydraulic conductivity (cm/sec)		4×10^{-5}	1×10^{-3}
Plasticity index (%)	D-4318	39	--
Liquid limit (%)	D-4318	76	--

Note: water content was measured as the weight of water/weight of solids

where f_{oc} is the organic carbon fraction and K_{oc} is the organic carbon partitioning coefficient, and the values are reported in Table 1. Myers *et al.* (1996) conducted laboratory diffusion experiments to estimate the partitioning coefficients for TCDD with the sediment and capping materials used in this study. The estimated partitioning coefficient agrees with reported values of Myers *et al.* (1996). For this analysis, we assumed that the initial concentration of TCDD in the model was equal to the maximum advected into the pore water concentration at the end of the centrifuge test. The seepage velocity was estimated to be 2.3×10^{-3} cm/sec from the hydraulic conductivity and the porosity provided in Table 2. The hydrodynamic dispersion coefficient, D_A, was estimated from the graphs of the dimensionless dispersion coefficient versus the Peclet number (i.e. $v\,d/D_d = 7$) given by Perkins and Johnson (1963). From this graph, the longitudinal and transverse dispersion coefficients for the cap were estimated to be 1×10^{-5} cm^2/sec and 4×10^{-6} cm^2/sec, respectively.

3.1 Capping thickness

Sensitivity analysis of Eq. 5 was conducted on the contaminant transport parameters. The partitioning coefficient of the cap was held constant. Figure 2 shows the effect of capping thickness on the predicted TCDD concentration from Eq. 5. For the estimated parameters for the centrifuge test (where v = 1×10^{-3} cm/sec and $D_a = 1\times10^{-5}$ cm^2/sec), as the cap thickness decreases the time to breakthrough decreases. For the estimated parameters, the advection-dispersion equation predicts a plug flow phenomena.

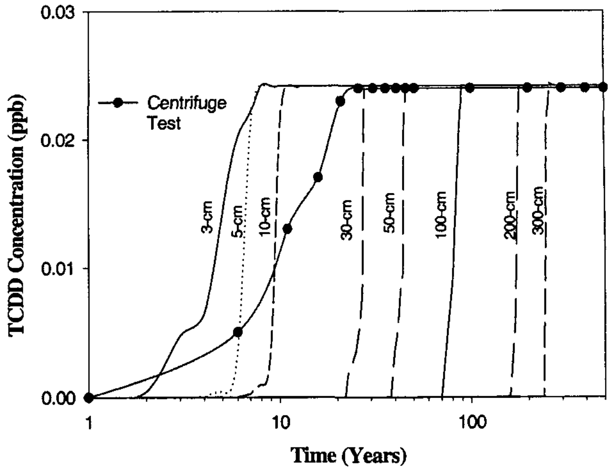

Fig. 2. Effects of cap thickness on TCDD breakthrough curves.

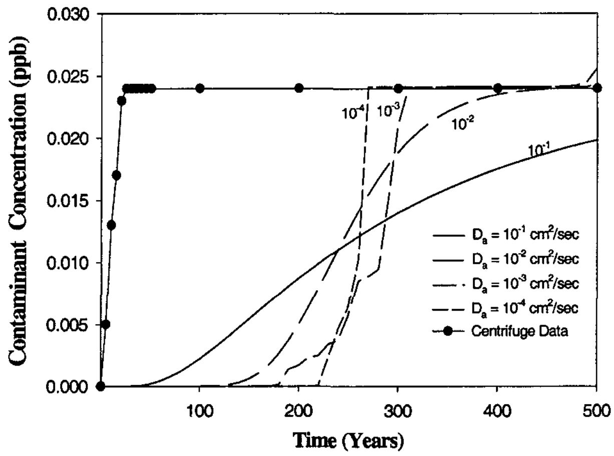

Fig. 3. Effects of hydrodynamic dispersion on TCDD breakthrough curve.

3.2. Hydrodynamic dispersion

Figure 3 shows the effects of hydrodynamic dispersion on the predicted TCDD concentration from Eq. 5. For a cap thickness of 300 cm and a velocity of 1×10^{-3} cm/sec, the advection dispersion equation overestimates the breakthrough time. As the hydrodynamic dispersion increases, the breakthrough time increased.

3.3 Velocity

Figure 4 shows the effects of velocity on the predicted breakthrough concentration of TCDD from Eq. 5. As the velocity increases (where z = 300 cm and $D_a = 1\times10^{-5}$ cm^2/sec), the breakthrough time for TCDD decreased. For the estimated parameters, Eq. 5 predicts a plug flow phenomena.

Figure 5 shows the fitted parameters for Eq. 5 where the velocity and hydrodynamic dispersion coefficients are estimated to be 1×10^{-2} cm/sec and 1×10^{-2} cm^2/sec. The fitted velocity and hydrodynamic dispersion were one and three orders of

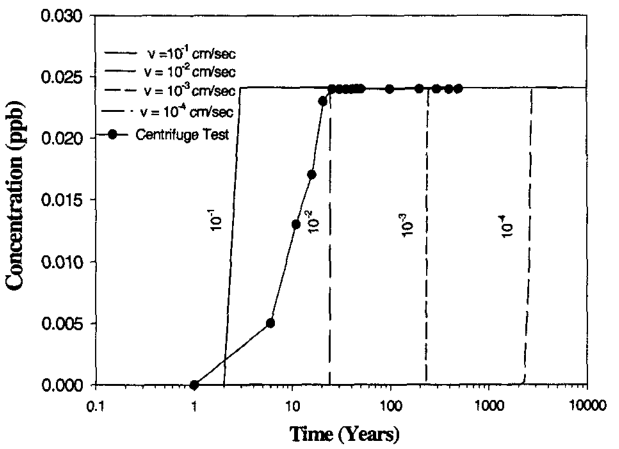

Fig. 4. Effects of velocity on TCDD breakthrough curve.

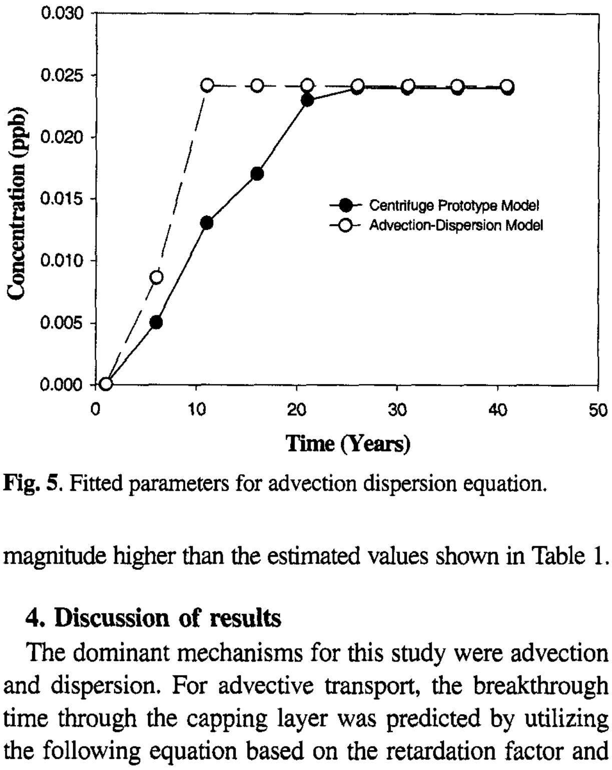

Fig. 5. Fitted parameters for advection dispersion equation.

magnitude higher than the estimated values shown in Table 1.

4. Discussion of results

The dominant mechanisms for this study were advection and dispersion. For advective transport, the breakthrough time through the capping layer was predicted by utilizing the following equation based on the retardation factor and the assumption of instantaneous sorption:

$$t_b = \frac{LR_f}{v} \tag{7}$$

where L is the length of the capping layer[5]. The predicted breakthrough time for the capping layer was 6.15 years (where L = 300 cm, K_d = 6471, and $v_{fitted} = 1\times10^{-2}$ cm/sec). The time for complete breakthrough in the centrifuge prototype is approximately 25 years. This indicates that the advective-dispersion transport in the centrifuge was the dominant phenomena. This conclusion is also supported by the relationship between the ratio of the hydrodynamic dispersion to molecular diffusion (i.e. $D_{afitted} = 1\times10^{-2}$ cm^2/sec, and $D_d = 5.6\times10^{-6}$ cm^2/sec and ratio = 1800) and Peclet number, which illustrates that advection-dispersion is the dominant transport process in this centrifuge study[7].

In addition, TCDD is a hydrophobic organic compound with a high partitioning coefficient. The breakthrough time predicted by Eq. 5 is based on the retardation of the contaminant. Based on the partitioning coefficient for the sediment which was estimated from the octanol-water partitioning coefficient and the organic fraction, the estimated aqueous concentration of TCDD is 2.4×10^{-4} μg/l, which is two orders of magnitude lower than the observed TCDD concentration in the centrifuge test. It seems that the centrifuge test is sensitive to sorption. Further testing is required to determine if there is a relationship between centrifuge gravitational acceleration and sorption phenomena.

Arulanandan *et al.* (1988) indicated that advective transport can be simulated even if the dispersion coefficient is violated. In addition, since the dispersion coefficient becomes larger in the model than in the prototype, the transport due to dispersion is faster in the model. This error is on the conservative side when considering the transport of pollutants. In this study, the centrifuge modeling results are considered non-conservative.

5. Summary and Conclusions

In the previous paper[4], centrifuge tests were conducted to determine the significance of consolidation induced advective transport of radiolabeled organic contaminants through a cap, and test results indicated that advection and dispersion are the dominant transport processes. In this study, the centrifuge test result was compared to the advection dispersion equation to predict contaminant transport parameters. Sensitivity analysis was also conducted on the advection dispersion equation.

The fitted contaminant transport parameters for the centrifuge test results were one to three orders of magnitude greater than the estimated parameters. This indicates that the centrifuge test over estimated the contaminant transport phenomena where breakthrough times in the centrifuge were greater than the advection dispersion equation. Thus, the centrifuge provides a non-conservative approach to modeling contaminant transport in this study. As the cap thickness decreased or the velocity increased, the breakthrough time decreased.

It should be noted that the advection dispersion equation used in this study is a one layered model. Two layered modeling approaches are more appropriate for modeling this data since there are two layers with different partitioning coefficients. Further research is required to model the centrifuge test using two-layered advection-dispersion models. Moreover, a comprehensive mathematical model that couples contaminant transport and consolidation is needed to verify centrifuge results.

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