Contamination of An Isolation Cap Due to Retardation

a report to the
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on the

Housatonic River Project

by
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Introduction

Retardation of transport occurs with many contaminants, including PCBs. PCBs have relatively large retardation factors, which may be on the order of tens of thousands. These large retardation factors are frequently used in transport modeling of aqueous processes; but the impact on the porous medium is often neglected. The importance of considering this impact is clear from the conservation of mass. As the contaminant transport within the pore water is being retarded, the receptor sites within the porous medium are being filled. The rate of accumulation of contaminant within the porous medium is a direct and inescapable result of the retardation.

Development

The rate of increase of the contaminant in the porous medium is equal to the flux of contaminant into the medium less the flux leaving the medium. The governing partial differential equation for the aqueous concentration, C_a, is given by Equation 1:

$$\frac{\partial C_a}{\partial t} = D_a \frac{\partial^2 C_a}{\partial x^2} - \frac{V}{\Re} \frac{\partial C_a}{\partial x} \tag{1}$$

where t is the temporal variable (time), x is the spatial variable (position), D_a is the diffusion coefficient for the contaminant in water, V is the advective velocity, and $\mathcal{R}$ is the retardation factor. Conservation of mass requires that the partial differential equation for the corresponding process in the porous medium, C_m, be given by Equation 2:

$$\frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial x^2} - \frac{V}{(1-\varepsilon)} \left(1 - \frac{1}{\Re} \right) \frac{\partial C_a}{\partial x} \tag{2}$$

where D_m is the diffusion coefficient for the contaminant in the porous medium and ε is the porosity. As the retardation factor, $\mathcal{R}$, approaches 1, there is no retardation and no accumulation of the contaminant in the porous medium. As the retardation factor approaches infinity, all of the contaminant leaves the porewater and fills the receptor sites in the porous medium. As the porosity approaches 0, all of the volume is available as the porous medium. As the porosity, ε, approaches 1, the porous medium occupies none of the total volume; thus, any presence of a contaminant would be an infinite concentration.

Results

An example is given to illustrate the magnitude of the quantities involved. Consider the case where the thickness of the isolation cap, L_i, is 2 feet, the advective velocity, V, is 100 ft/yr, the initial (entering) concentration in the porewater, C_0, is 0.009 ppm, the porosity, ε, is 0.3, both diffusion coefficients, D_a and D_m, are 0.034 ft²/yr, and the retardation factor, $\Re$, is 100. Equation 1 can be solved analytically.

$$C_a = \frac{C_0}{2} erfc\left(\frac{x - \frac{Vt}{\Re}}{2\sqrt{D_a t}}\right) \tag{3}$$

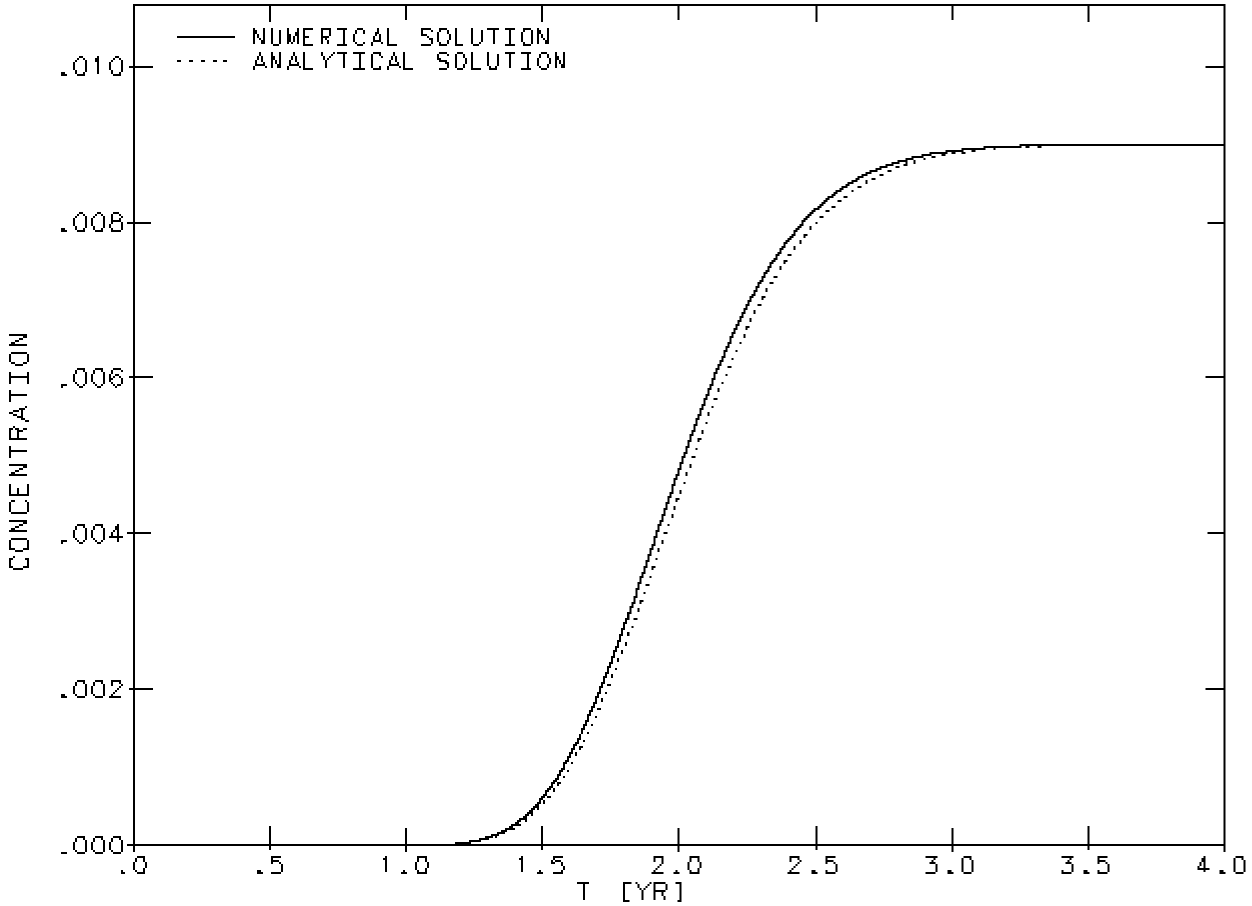

Figure 1. Porewater Concentration History at X = 2 Feet

Equation 2 cannot be solved analytically; therefore, a numerical solution will be used. Figures 1 and 2 show the agreement between the analytical and numerical solutions to Equation 1. Figure 1 is the porewater history (concentration vs. time) at the end of the isolation layer. Figure 2 is the porewater profile (concentration vs. location) at a selected time.

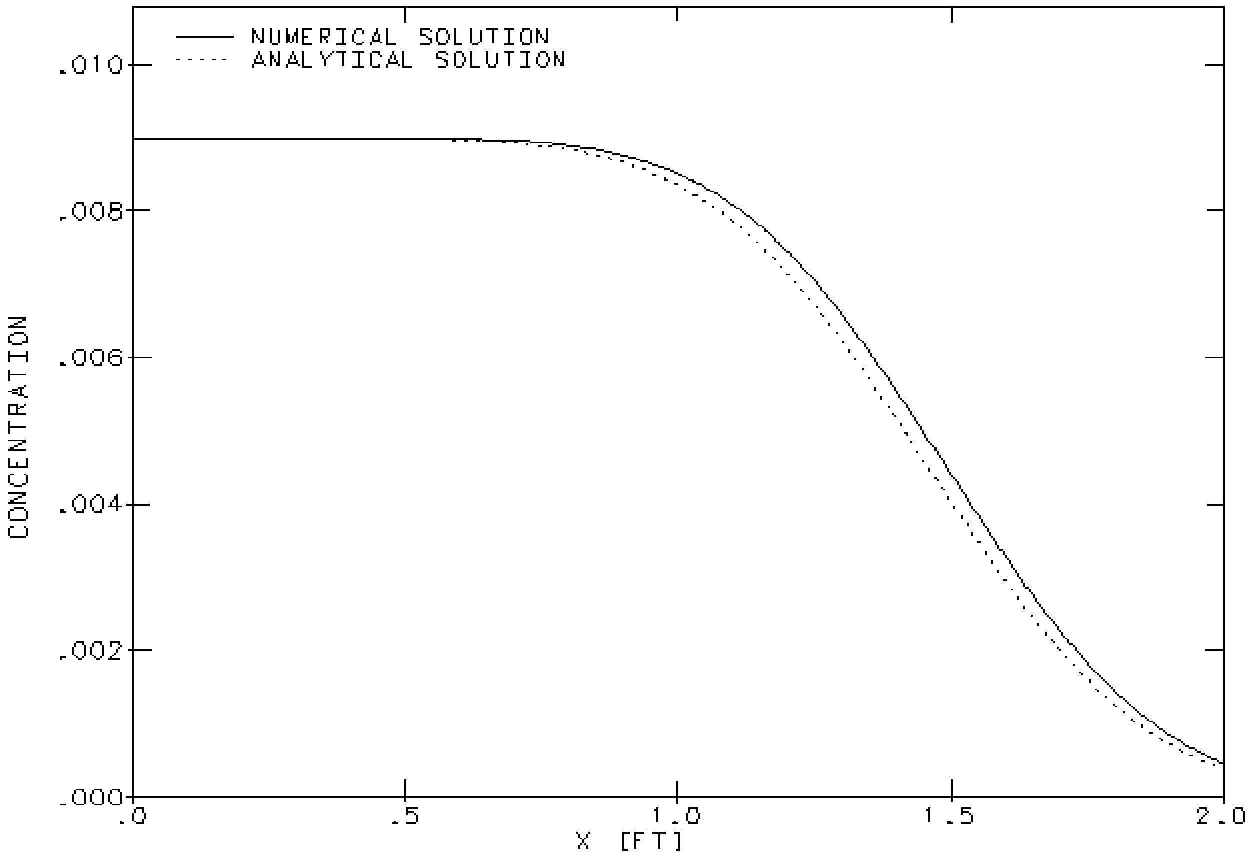

Figure 2. Porewater Profile at T = 1.46 Years

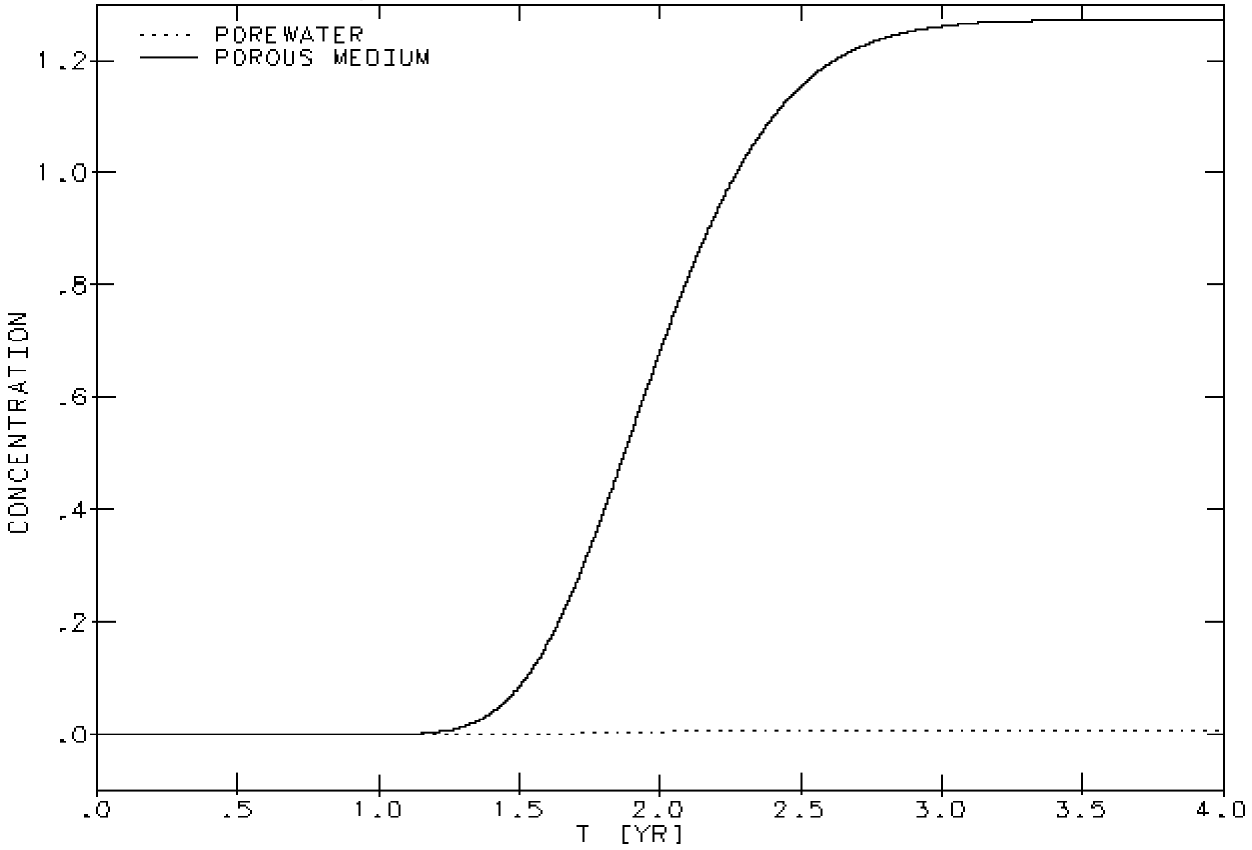

Figure 3. Porous Medium History at X = 2 Feet

The agreement between the numerical and analytical solutions is evident from these two plots. The porous medium side of the process, Equation 2, was solved numerically at the same time. Figures 3 and 4 show the porous medium history and profile.

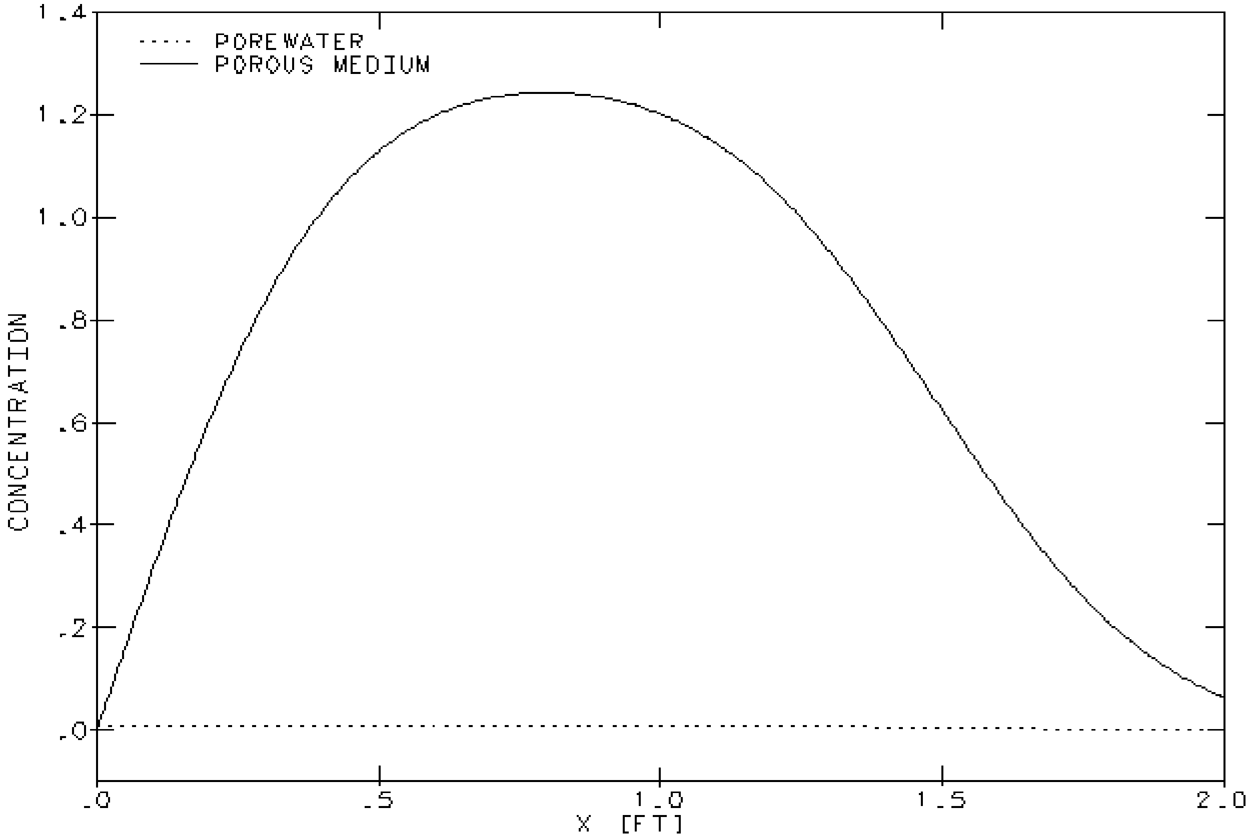

Figure 4. Porous Medium Profile at T = 1.46 Years

It is clearly evident from Figures 3 and 4 that the conservation of mass necessitates that retardation result in a proportional increase in concentration in the porous medium. These calculations were made with a retardation factor of 100. The impact would be 300 times as great were the retardation factor 30,000, which some geohydrologists insist is appropriate in this case.

Conclusion

If the isolation cap performs as designed, it will retain a significant amount of the contaminant when the leading edge breaks through the cap.

Symbols

C_0	initial (entering) concentration in the porewater
C_a	concentration in the porewater
C_m	concentration in the porous medium
D_a	diffusion coefficient for the contaminant in water
D_m	diffusion coefficient for the contaminant in the porous medium
L_i	thickness of the isolation layer
t	temporal variable (time)
V	advective velocity
x	spatial variable (position)
ε	porosity
$\mathfrak{R}$	retardation factor

References

Wu, S. C. and P. M. Gschwend, 1988, "Numerical Modeling of Sorption Kinetics of Organic Compounds to Soil and Sediment Particles," *Water Resources Research*, Vol. 24, No. 8, pp. 1373-1383.

Wu, S. C. and P. M. Gschwend, 1986, "Sorption Kinetics of Hydrophobic Organic Compounds to Natural Sediments," *Environmental Science Technology*, Vol. 20, No. 7, pp. 717-725.