ground water

Containment Criterion for Contaminant Isolation by Cutoff Walls

by Christopher J. Neville[1] and Charles B. Andrews[2]

Abstract

A rigorous solution is developed from first principles to guide the preliminary design of cutoff walls installed to contain the migration of contaminants from source zones. The full analytic solution is used to develop a criterion for determining the configuration and hydraulics of optimal wall designs. The solution is used to demonstrate the interaction between the properties of the wall, the Darcy flux, and the concentration of contaminants at the outside face of the well. For a particular wall design, the containment criterion can be used to estimate the long-term concentration that will develop at the outside face of the wall. Alternatively, for a given concentration on the outside face of the cutoff wall, the containment criterion can be used to estimate the Darcy flux required to balance the outward diffusion of contaminants. The results of numerical simulations are presented to evaluate the analytic approach. The numerical results confirm that for a wall with known transport properties, a specified Darcy flux is associated with a unique outside contaminant concentration.

Introduction

Cutoff walls composed of soil-bentonite slurries have been used for ground water control in geotechnical applications since ~1945 (Jefferis 1997). More recently, cutoff walls have become a key component of remedial systems at hazardous waste sites to isolate the source area and thereby hasten the cleanup of downgradient plumes (Rumer and Ryan 1995). Assessments of slurry wall technology and reviews of environmental applications are presented by Ryan (1985), Turchan et al. (1989), and Rumer and Mitchell (1995).

Design specifications for cutoff walls for contaminant isolation have traditionally been expressed in terms of maximum permissible hydraulic conductivities (Spooner et al. 1984). This design basis presumes that advection is the only solute transport process of significance. In contrast, Shackelford (1988) and Rowe et al. (1995) among others have demonstrated that diffusion is the dominant transport process across a properly constructed low-conductivity wall. Consideration of the interaction between the processes of advection and diffusion should be an integral part of cutoff wall design.

In addition to analyzing the hydraulics of a proposed wall configuration, contaminant transport modeling is required to support the selection of wall materials, to select the wall thickness, and to guide performance monitoring. Rumer and Mitchell (1995, chap. 10) provide a thorough review of analysis methods for transport across low-permeability barriers. Khandelwal et al. (1997) and Rabideau and Khandelwal (1998) developed a general semianalytic approach for the prediction of contaminant concentration profiles across barriers. As part of a larger analysis of optimal barrier designs, Devlin and Parker (1996) developed a containment criterion for a cutoff wall, starting from the condition that the mass fluxes across the wall be in balance. Devlin and Parker (1996) suggested that the optimum hydraulic conductivity is not the lowest value but that value that gives rise to the minimum outward mass flux.

Although comprehensive analytic and numerical methods are available for predicting the performance of cutoff walls, there remains the need for simple closed-form solutions that can be used for preliminary design

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calculations. In this paper, the problem of steady transport across a cutoff wall is analyzed from first principles. An analytic solution is developed to demonstrate that transport across a wall is intimately related to the contaminant concentration at the outside face of the wall. The solution is used to develop a physically based criterion for determining the configuration and hydraulics of optimal cutoff wall designs. Numerical simulations are conducted to check the predictions of the containment criterion.

Analytic Solution for Steady Transport across a Cutoff Wall

The conceptual model for transport across a cutoff wall is shown in Figure 1. The following primary assumptions are invoked in the analysis: the material properties of the wall are uniform; ground water flow is steady, uniform, and one-dimensional; and sufficient time has elapsed that a steady concentration profile has developed across the wall. It is also assumed that the solute is nonreactive. For steady-state conditions, the statement of mass conservation for a nonreactive solute is written as:

$$0 = -\frac{\mathrm{d}}{\mathrm{d}x}(J_{\mathrm{A}}) - \frac{\mathrm{d}}{\mathrm{d}x}(J_{\mathrm{D\,mech}}) - \frac{\mathrm{d}}{\mathrm{d}x}(J_{\mathrm{D\,diff}}) \tag{1}$$

where J_{A}, $J_{\mathrm{D\ mech}}$, and $J_{\mathrm{D\ diff}}$ are the advective, dispersive, and diffusive mass fluxes, respectively. The mass fluxes are defined as:

$$J_{\mathrm{A}} = qc \tag{2}$$

$$J_{\mathrm{D\,mech}} = -\phi\alpha_{\mathrm{L}}\frac{|q|}{\phi}\frac{\mathrm{d}c}{\mathrm{d}x} \tag{3}$$

$$J_{\mathrm{D\,diff}} = -\phi D^{*}\frac{\mathrm{d}c}{\mathrm{d}x} \tag{4}$$

where c is concentration [ML^{-3}], q is Darcy flux [LT^{-1}], ϕ is the effective porosity for transport [dimensionless], α_{L} is longitudinal dispersivity [L], and D^{*} is the effective molecular diffusion coefficient [$\mathrm{L}^2\mathrm{T}^{-1}$].

The dispersive mass flux is written using the one-dimensional form of the dispersion tensor adopted by Bear (1972) and Burnett and Frind (1987). It is important to note that the dispersion coefficient is defined in terms of the absolute value of the Darcy flux. According to the Fickian model, the dispersive and diffusive mass fluxes act in the same direction and are always directed opposite to the concentration gradient, regardless of the direction of the Darcy flux (a positive gradient is defined here as being in the direction of increasing concentration). In Figure 1, the highest concentration is the source concentration within the barrier, c_0. As shown in Figure 1, for this case the diffusive mass flux is always directed outward from the source zone, regardless of the direction of ground water flow. This is also the case for the mechanical dispersive mass flux. This model of dispersion has been incorporated in most general solute transport simulators, including MOC3D (Konikow et al. 1996), MT3D^{99} (Zheng and SSP&A 1999), and MODFLOW-SURFACT (HydroGeoLogic Inc. 1996).

The final form of the governing equation is obtained by substituting for the definitions of the mass fluxes in Equation 1 and invoking the assumption of uniform material properties:

$$\begin{aligned} 0 &= -q\frac{\mathrm{d}c}{\mathrm{d}x} + \phi\alpha_{\mathrm{L}}\frac{|q|}{\phi}\frac{\mathrm{d}^2c}{\mathrm{d}x^2} + \phi D^{*}\frac{\mathrm{d}^2c}{\mathrm{d}x^2} \\ &= -q\frac{\mathrm{d}c}{\mathrm{d}x} + \phi D\frac{\mathrm{d}^2c}{\mathrm{d}x^2} \end{aligned} \tag{5}$$

where D designates the coefficient of hydrodynamic dispersion defined as:

$$D = \alpha_{\mathrm{L}}\frac{|q|}{\phi} + D^{*} \tag{6}$$

Boundary conditions are required at the inside and outside faces of the slurry wall. The contaminant source is represented as a constant-concentration boundary condition at the inside face of the wall:

$$c(x = 0) = c_0 \tag{7a}$$

The stabilization of concentrations requires that the contaminant concentration on the outside face of the wall also reach a constant value; therefore, the boundary condition on the outside face of the wall is written as:

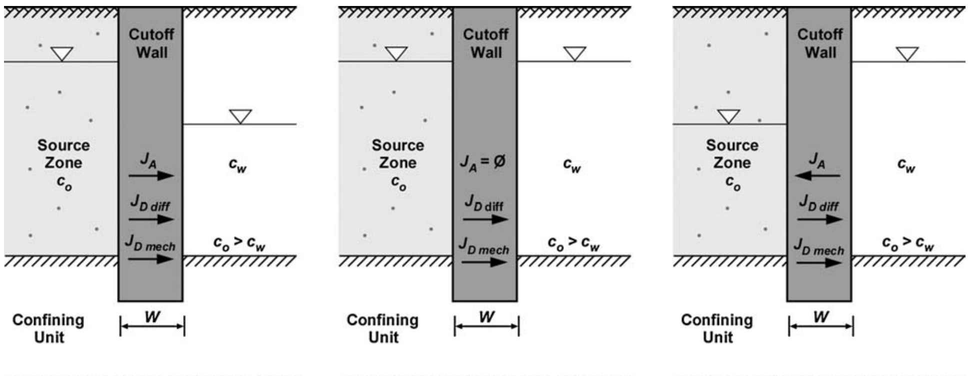

Figure 1. Conceptual configurations of a cutoff wall illustrating advective, diffusive, and mechanical dispersive fluxes when (a) water level inside the wall is higher than that outside the wall, (b) water level inside the wall is the same as that outside the wall, and (c) water level inside the wall is lower than that outside the wall (after Manassero and Pasqualini 1993).

$$c(x = w) = c_w \tag{7b}$$

The analytic solution of Equation 5 subject to Equation 7 is:

$$c = c_0 - (c_0 - c_w)\left[\frac{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)x\right\}}{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)w\right\}}\right]; \quad q \neq 0 \tag{8}$$

Equation 8 holds for all nonzero values of the Darcy flux. The solution for purely dispersive transport is:

$$c = c_0 - (c_0 - c_w)\frac{x}{w}; \quad q = 0 \tag{9}$$

The behavior of the solution is illustrated with some example calculations. The following parameter values are assumed: wall thickness, $w = 1.0$ m; effective porosity, $\phi = 0.3$; longitudinal dispersivity, $\alpha_L = 0.01$ m; and effective molecular diffusion coefficient, $D^* = 3.0 \times 10^{-6}$ cm^2/s. The relative concentration at the outside face of the wall, c_w/c_0, is fixed at a value of 0.01. Concentration profiles across the wall are plotted in Figure 2 for five values of the Darcy flux, including flows both into and out of the wall.

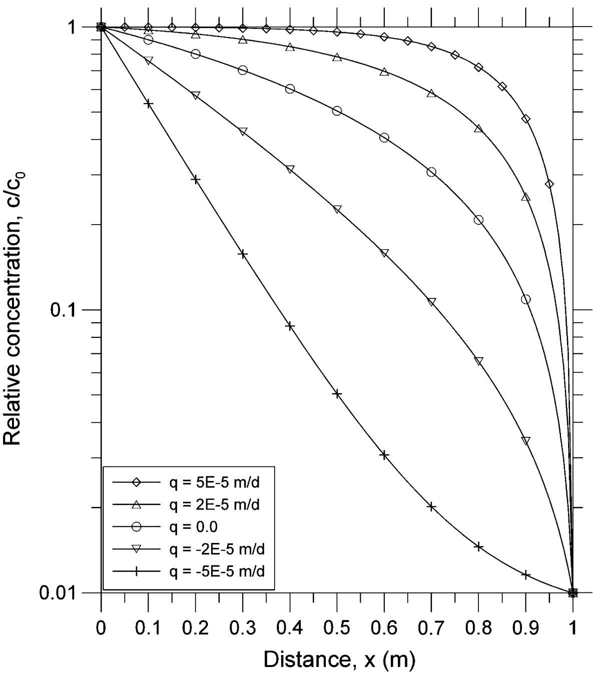

Figure 2. Calculated concentration profiles.

Containment Criterion for a Cutoff Wall

The results shown in Figure 2 illustrate that Equation 7 yields physically admissible results for all values of the Darcy flux. To obtain a workable criterion for cutoff wall design, Devlin and Parker (1996) imposed the constraint that the net mass flux out of the wall be zero. This constraint can be expressed as:

$$0 = J_A + (J_{D\,\mathrm{mech}} + J_{D\,\mathrm{diff}}) \tag{10}$$

Expressions for the advective mass flux J_A and the sum of the dispersive and diffusive fluxes, J_D, are derived by substituting the solution for the concentration into Equations 2, 3, and 4:

$$J_A = qc = q\left[c_0 - (c_0 - c_w)\frac{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)x\right\}}{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)w\right\}}\right] \tag{11}$$

$$J_D = -\phi D\frac{\mathrm{d}c}{\mathrm{d}x} = -q(c_0 - c_w)\left[\frac{\mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)x\right\}}{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)w\right\}}\right] \tag{12}$$

The expressions for the fluxes at the outside face of the wall are obtained by evaluating Equations 11 and 12 at $x = w$:

$$J_A = qc_w \tag{13}$$

$$J_D = -q(c_0 - c_w)\left[\frac{\mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)w\right\}}{1 - \mathrm{EXP}\left\{\left(\frac{q}{\phi D}\right)w\right\}}\right] \tag{14}$$

Setting $J_A + J_D = 0$ and solving for c_w yields:

$$\frac{c_w}{c_0} = \mathrm{EXP}\left\{\frac{qw}{\phi D}\right\} \tag{15}$$

Equation 15 is plotted in Figure 3. The line represents the boundary between regions of net inward and net outward mass flux. Figure 3 may be used in several ways. For a given wall design expressed in terms of the ratio $qw/\phi D$, the plot can be used to estimate the long-term concentration that will develop at the outside face of the wall. The plot can also be used to estimate the Darcy flux required to balance the outward diffusion of the contaminant for a given concentration on the outside face of the wall. The results plotted in Figure 3 show that for inward flows ($q < 0$), the stabilized concentration c_w increases toward c_0 as the absolute value of the Darcy flux decreases. The results also show that for a given negative Darcy flux, the stabilized concentration on the outside of the wall increases as the thickness of the wall is decreased.

Evaluation of the Containment Criterion

The concentration at the inside and outside faces of the wall was fixed a priori in the analytic solution. It is possible to fix both the Darcy flux and the contaminant concentration at the outside face of the wall under controlled laboratory conditions (see, for example, Rowe et al. 2000). Similar conditions have been invoked in the back-analysis of solute profiles that have evolved over geologic time scales (for example, Desaulniers et al. 1986). In field-scale applications, only the Darcy flux across the cutoff wall can be controlled, and the concentration outside of the wall will evolve. Numerical simulations have been developed to confirm that the containment criterion is meaningful in general. The

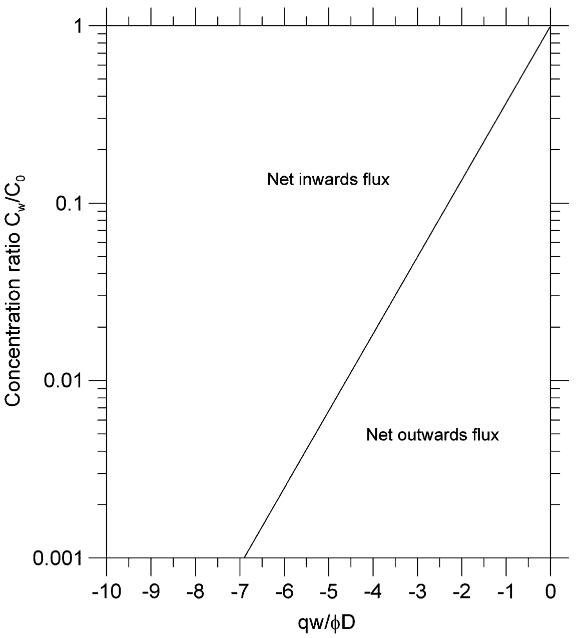

Figure 3. Conditions for zero net mass flux at outside face of wall.

simulations are conducted with the comprehensive numerical flow and transport simulators MODFLOW (McDonald and Harbaugh 1988) and MT3D^{99} (Zheng and SSP&A 1999).

The numerical model comprises three segments: a reservoir representing the source zone, the slurry wall, and an outer zone representing the aquifer that has been isolated from the source. The source zone has a length of 0.1 m and is assigned a constant-concentration condition in the transport model and a constant-head condition with respect to ground water flow. The specified head is adjusted to vary the Darcy flux across the wall. The cutoff wall is 1.0 m long and is divided into 10 blocks. The outer zone representing the aquifer zone is divided into eleven 0.1-m-long blocks. Solute is free to leave the domain at the end of the mixing zone through a zero-gradient boundary condition imposed in conjunction with a constant-head condition. The transport model as structured does not impose a fixed-concentration condition at the outside face of the slurry wall. An effective diffusion coefficient of 3×10^{-6} cm^2/s and a porosity of 0.3 are assumed for all simulations.

The MT3D^{99} simulations have been evaluated with implicit time weighting using the generalized conjugate gradient solver package. Particular care has been taken to ensure that the MT3D^{99} simulations are as free of numerical artifacts as possible. All simulations have been repeated using two methods to approximate the advection term: finite-difference and third-order ULTIMATE. The finite-difference solutions have been evaluated using both upstream and centered-in-space weighting of the advection term, satisfying the Courant constraint at all times. The mass balance discrepancy was <0.1% in all simulations.

The calculated breakthrough curves outside of the wall are plotted in Figure 4. When the Darcy flux, *q*, is zero, or directed outwards from the source, the concentration outside of the wall eventually attains the level of the source concentration. In contrast, when there is an inward Darcy flux, the concentration stabilizes at some fraction of the source concentration. The stabilized contaminant concentration decreases for progressively larger inward Darcy fluxes. The stabilized concentrations calculated with MT3D^{99} are relatively close to the results of the analytic solution, indicated by the dashed lines. The good agreement between the analytic and numerical results demonstrates the containment criterion is applicable for long-term conditions, provided that hydraulic conditions and the properties of the wall remain constant. The numerical results confirm that for a wall with known transport properties, a specified Darcy flux is associated with a unique outside contaminant concentration.

Conclusions

An analysis of the transport of contaminants across a cutoff wall has demonstrated that transport is intimately related to the contaminant concentration at the outside face of the wall. An analytic solution has been developed as the foundation for a physically based criterion for determining the configuration and hydraulics of optimal slurry wall designs. For a particular wall design, the containment criterion can be used to estimate the long-term concentration that will develop at the outside face of the wall. Alternatively, for a given concentration on the outside face of the cutoff wall, the containment criterion can be used to estimate the Darcy flux required to balance the outward diffusion of contaminants. Calculations made with the containment criterion have been checked against results from simulations with a comprehensive numerical model. The agreement between the numerical and analytic results confirms the predicted relations between the Darcy flux and the long-term concentration of contaminants at the outside face of a cutoff wall.

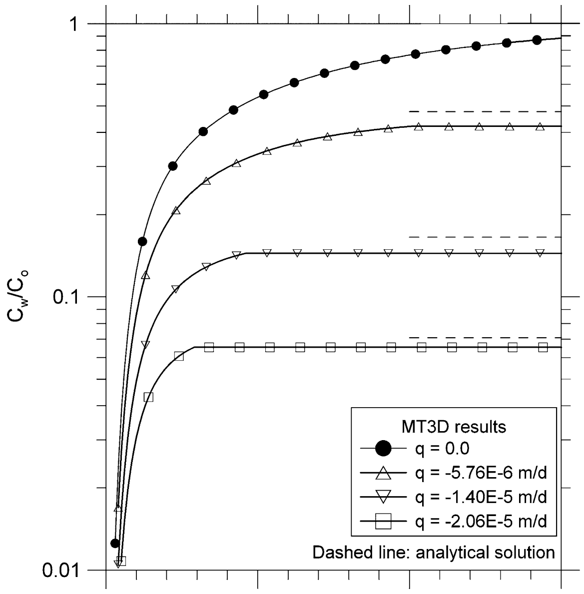

Figure 4. Comparison of stabilized concentrations at the outside face of the wall predicted by the numerical and analytic solutions.

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