

BIOSCREEN-AT: BIOSCREEN with an Exact Analytical Solution

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Abstract

BIOSCREEN is used extensively for screening-level evaluation of the transport of dissolved contaminants in ground water. The code has an effective graphical user interface that makes it ideal for use in both professional practice and as a teaching aid. BIOSCREEN implements the approximate transport solution of Domenico (1987). This note describes an enhanced version of the program, BIOSCREEN-AT, which supplements the Domenico solution with an exact analytical solution. The exact analytical solution has been integrated seamlessly within the BIOSCREEN interface and provides a simple and direct way to calculate an exact solution to the transport equation and, if desired, to assess the significance of the errors introduced by the Domenico (1987) solution for site-specific applications. The modified version of BIOSCREEN is designated BIOSCREEN-AT and can be downloaded free of charge from <http://www.sspa.com/.software/BIOSCREEN.htm>.

Introduction

BIOSCREEN is a screening-level model developed for and distributed by the U.S. EPA (Newell et al. 1997) that simulates remediation through natural attenuation of dissolved hydrocarbons at petroleum fuel release sites. BIOSCREEN is also used extensively for simulating the movement of a wide variety of solutes in ground water. The program is implemented in the Microsoft Excel™ spreadsheet environment, which provides an effective interface that is ideal for use in both professional practice and as a teaching aid. BIOSCREEN implements the Domenico solution for solute transport in three-dimensional porous media (Domenico 1987; Martin-Hayden and Robbins 1997). The Domenico model has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions that have been shown to be the dominant biodegradation processes at many petroleum release sites.

Attention has recently been directed to the accuracy of the Domenico (1987) solution that is used to calculate

concentrations in BIOSCREEN. The Domenico (1987) solution was recognized from its inception as a heuristic solution that was approximate in nature. Guyonnet and Neville (2004) have shown that the Domenico (1987) solution may under some circumstances produce solutions that differ significantly from rigorous solutions to the same problem. This note describes an enhanced version of BIOSCREEN that supplements the Domenico (1987) solution with an exact analytical solution for the concentration. The exact solution is derived for the same conceptual model as Domenico (1987) but without invoking approximations in its evaluation that introduce errors of unknown magnitude in the analysis.

The exact analytical solution is integrated seamlessly within a modified interface BIOSCREEN-AT. The Excel user interface for BIOSCREEN-AT is nearly identical to that for BIOSCREEN, and a user familiar with BIOSCREEN will have no difficulty using BIOSCREEN-AT. BIOSCREEN-AT provides a simple and direct way to calculate an exact solution to the transport equation and, if desired, to assess the significance of the errors introduced by the Domenico (1987) solution for site-specific applications.

Exact Analytical Solution

The conceptual model for the BIOSCREEN model is shown in Figure 1. The aquifer is assumed to be semi-infinite in extent in the *x*-direction, infinite in extent in

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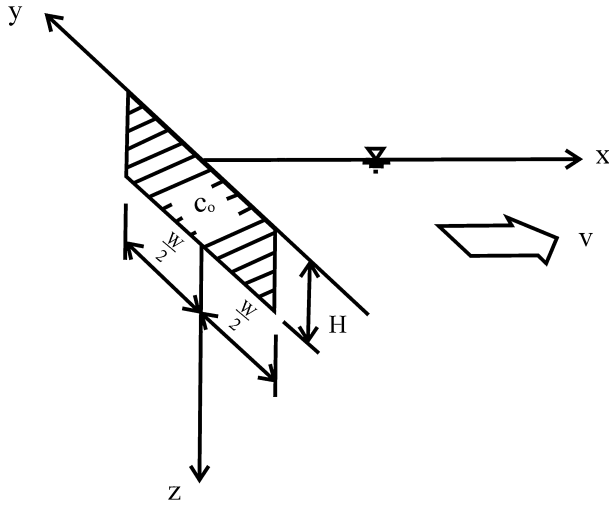


Figure 1. Conceptual model.

the y -direction, and extending from the water table to a relatively large depth. Ground water flow is steady and one dimensional. The source is represented as a patch specified-concentration boundary condition along the inflow boundary. Solute transport across the patch is by advection and three-dimensional dispersion, and the solute undergoes equilibrium sorption and first-order transformation reactions.

The governing equation for three-dimensional transport with steady, uniform ground water flow in the x -direction is:

$$R \frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} + D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - \lambda_{\text{EFF}} c \quad \text{over } 0 \leq x < \infty, -\infty < y < \infty, 0 \leq z < \infty \quad (1)$$

The terms used in all equations are defined in the Appendix. The term λ_{EFF} is a general decay term defined as:

$$\lambda_{\text{EFF}} = \lambda_D + \frac{\rho_b}{\theta} K_d \lambda_S \quad (2)$$

where λ_D and λ_S represent the first-order transformation rates in the dissolved and sorbed phases, respectively. The term λ_{EFF} is introduced to accommodate a range of assumptions regarding the relative magnitudes of the decay rates in the dissolved and sorbed phases. For example, for biodegradation reactions it is assumed frequently that transformations occur only in the dissolved phase (Criddle et al. 1991). The dispersion coefficients are adopted from Burnett and Frind (1987):

$$\begin{aligned} D_x &= \alpha_L |v| + D^*; D_y = \alpha_{\text{TH}} |v| + D^*; \text{ and} \\ D_z &= \alpha_{\text{TV}} |v| + D^* \end{aligned} \quad (3)$$

The boundary condition along the inflow, $x = 0$, is written as:

$$c(0, y, z, t) = c_0 \text{EXP}\{-\gamma t\} \left[U\left(y + \frac{W}{2}\right) - U\left(y - \frac{W}{2}\right) \right] \times [U(z) - U(z - H)] \quad (4)$$

where $U(\bullet)$ are the Heaviside step function terms, which serve to locate the source between $\frac{W}{2}$ and $z = 0$ and H :

$$U(\xi - \xi_0) = 0, \text{ if } \xi < \xi_0; U(\xi - \xi_0) = 1, \text{ if } \xi > \xi_0 \quad (5)$$

The remaining boundary and initial conditions are written as:

$$c(\infty, y, z, t) = 0 \quad (6)$$

$$c(x, \pm \infty, z, t) = 0 \quad (7)$$

$$\frac{\partial c}{\partial z}(x, y, 0, t) = 0, \quad c(x, y, \infty, t) = 0 \quad (8)$$

$$c(x, y, z, 0) = 0 \quad (9)$$

Integral transform techniques can be used to derive an exact solution (Cleary and Ungs 1978; Sagar 1982; Wexler 1992). The solution presented here is a generalization of the Sagar (1982) solution for a decaying influent concentration. The boundary condition at the water table is incorporated using image theory, with the patch of specified concentration extending over the depth $-H \leq z \leq +H$.

$$\begin{aligned} c(x, y, z, t) &= c_0 \frac{x}{8\sqrt{\pi D_x}} \text{EXP}\{-\gamma t\} \\ &\times \int_0^t \frac{1}{\xi^{3/2}} \text{EXP}\left\{(\gamma - \lambda_{\text{EFF}})\xi - \frac{(x - v'\xi)^2}{4D'_x \xi}\right\} \\ &\times \left[\text{ERFC}\left\{\frac{y - \frac{W}{2}}{2\sqrt{D'_y \xi}}\right\} - \text{ERFC}\left\{\frac{y + \frac{W}{2}}{2\sqrt{D'_y \xi}}\right\} \right] \\ &\times \left[\text{ERFC}\left\{\frac{z - H}{2\sqrt{D'_z \xi}}\right\} - \text{ERFC}\left\{\frac{z + H}{2\sqrt{D'_z \xi}}\right\} \right] d\xi \end{aligned} \quad (10)$$

where $v' = v/R$, $D'_x = D_x/R$; $D'_y = D_y/R$; and $D'_z = D_z/R$.

Additional notes containing the complete derivation of the solution and additional details on the application of image theory to account for the water table are included as supplementary materials available from the *Ground Water* Web site, <http://www.blackwell-synergy.com/loi/gwat>. The integral in the exact analytical solution is evaluated using standard Gauss-Legendre quadrature techniques (Press et al. 1992). The solution is implemented in a FORTRAN program that is included in a Dynamic Link Library in the BIOSCREEN-AT Excel user interface. The FORTRAN source code and compiled code for the complete implementation of the analytical solution, along with an example input and output file, are also included as supplementary materials available at the *Ground Water* web site.

Example Calculations

To demonstrate the application of the solution we compare the results between the Domenico (1987)

Table 1
Input Parameters for the Example Calculations

Parameter	Value
Average linear ground water velocity, v	10.0 m/yr
Longitudinal dispersivity, α_L	10.0 m
Horizontal transverse dispersivity, α_{TH}	0.5 m
Vertical transverse dispersivity, α_{TV}	0.05
Effective diffusion coefficient, D^*	0.0
Retardation factor, R	1.0
Effective first-order decay coefficient, λ_{EFF}	0.1386/year
Initial source concentration, c_0	1.0
Source decay coefficient, γ	0.0
Depth of source, H	2.0 m
Width of source, $2y_0$	20.0 m

solution and the exact solution and an alternative rigorous analytical solution. The Domenico solution is evaluated using BIOSCREEN v. 1.4. The exact solution is evaluated with both an independent implementation of the solution (ATRANS21) and the new program BIOSCREEN-AT. Results are also obtained with the analytical solution PATCH3D (Sudicky et al. 1988) that is incorporated in the MULTIMED program (Salhotra et al. 1995), a widely used screening program developed for the U.S. EPA. The PATCH3D solution is strictly applicable for aquifers that have finite thickness. For this comparison it is sufficient to ensure that the plume does not extend to the base of the aquifer. The input parameters for the example calculations are listed on Table 1. The solute decay rate λ_{EFF} corresponds to a half-life of 5 years.

Results are evaluated for a source concentration that is constant. As shown in Figure 2, the results obtained with BIOSCREEN-AT match the exact solution and PATCH3D. In contrast, the centerline concentrations calculated with the Domenico (BIOSCREEN) solution are lower. The errors in the BIOSCREEN calculations are case specific. In our opinion, the most important aspect of BIOSCREEN-AT is that it can be used to assess the magnitudes of the errors for particular cases.

BIOSCREEN-AT is a Microsoft Excel spreadsheet that is compatible with versions 2000 and later and can be downloaded free of charge from <http://www.sspa.com/software/BIOSCREEN.htm>.

Supplementary Material

The following supplementary material is available for this article:

Solution for transport from a patch boundary condition in an infinitely thick aquifer

This material is available as part of the online article from: <http://www.blackwell-synergy.com/doi/abs/10.1111/j.1745-6584.2006.00296.x>

(This link will take you to the article abstract).

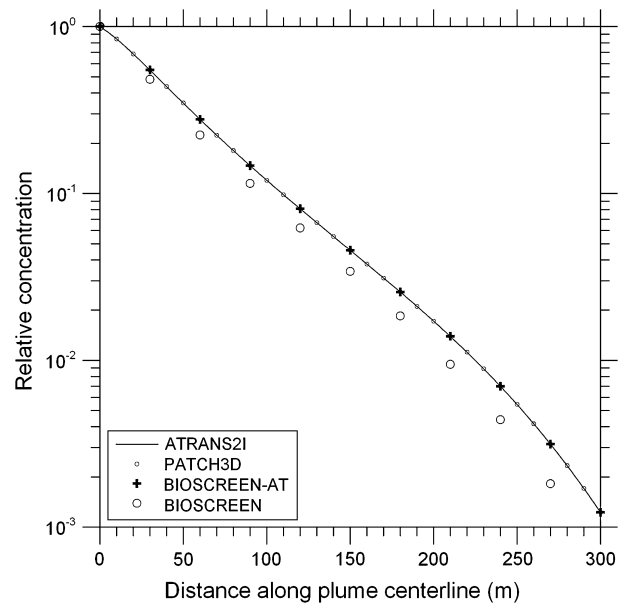


Figure 2. Calculated concentration profiles along plume centerline.

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Appendix: Notation

- x, y, z : spatial coordinates [L]
 t : time [T]
 c : dissolved concentration [ML^{-3}]
 θ : effective porosity (mobile water content) [–]
 ρ_b : bulk density [ML^{-3}]
 K_d : linear, equilibrium sorption coefficient [ML^{-3}]
 v : average linear ground water velocity [LT^{-1}]
 D_x, D_y, D_z : dispersion coefficients [L^2T^{-1}]
 λ_D : first-order transformation rate in the dissolved phase [T^{-1}]
 λ_S : first-order transformation rate in the solid phase [T^{-1}]
 α_L : longitudinal dispersivity [L]
 α_{TH} : horizontal transverse dispersivity [L]
 α_{TV} : vertical transverse dispersivity [L]
 D^* : effective diffusion coefficient [L^2T^{-1}]
 c_0 : initial source concentration
 R : retardation factor
 γ : source decay coefficient
 W : source width
 H : depth of penetration of the source below the water table.