GeoStudio Example File
Source and Exit Boundary Conditions

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Introduction

There are three basic boundary conditions for the divergence form of the contaminant transport equation: (1) specified concentration (Dirichlet), (2) specified normal dispersive and advective flux (Neumann) and (3) specified concentration and normal dispersive and advective flux (Cauchy). In many cases, these boundary conditions are sufficient and easily defined. For example, a contaminant source could be specified using either the Dirichlet (constant concentration) or Neumann (constant mass flux) type boundary condition. In transport analyses, however, the plume often reaches the far-field boundary, in which case none of these boundary conditions apply. Frind (1988) formulated a free exit (Cauchy) boundary condition that allows mass to exit by both advection and dispersion while responding to the changing concentration at the boundary. The free exit (Cauchy) boundary condition implemented in GeoStudio only allows mass to leave by advection.

The objectives of this example are to: (1) demonstrate the use of the constant and source concentration boundary conditions, (2) demonstrate the use of the solute free exit mass flux and solute mass flux boundary conditions, and (3) compare the results from GeoStudio to a closed-form solution of the advection-dispersion equation in a semi-infinite medium.

Background

Frind (1988) presents the following closed-form analytical solution to the convective form of the advection-dispersion equation for a one-dimensional semi-infinite medium with a Cauchy source boundary condition:

$$C = \frac{C_o}{2}\left[\left(erfc\left(\frac{x - vt}{2\sqrt{Dt}}\right) - exp\left(\frac{vx}{D}\right) erfc\left(\frac{x + vt}{2\sqrt{Dt}}\right)\left(1 + \frac{v(x + vt)}{D}\right)\right) + \frac{v\sqrt{t}}{\sqrt{\pi D}} exp\left(-\frac{(x - v}{4Dt}\right.\right. \quad \textbf{Equation 1}$$

where C is the concentration, C_o is the specified concentration in the source boundary, D is the hydrodynamic dispersion coefficient, v is the average linear velocity, t is the elapsed time, x is the distance from the source boundary, and $erfc$ is the complementary error function.

Numerical Simulation

Figure 1 presents the one-dimensional model domain. The GeoStudio Project, shown in Figure 2, includes a steady-state water transfer analysis and three transient solute transfer analyses. As shown in Figure 3, the advection-dispersion physical process is selected in all transport analyses.

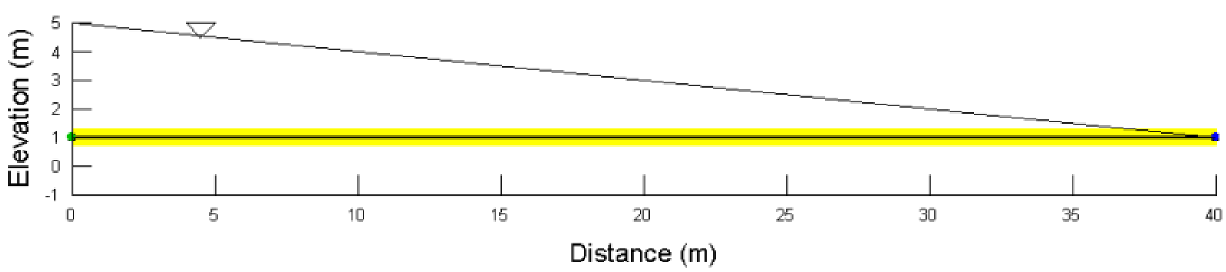

Figure 1. Problem configuration.

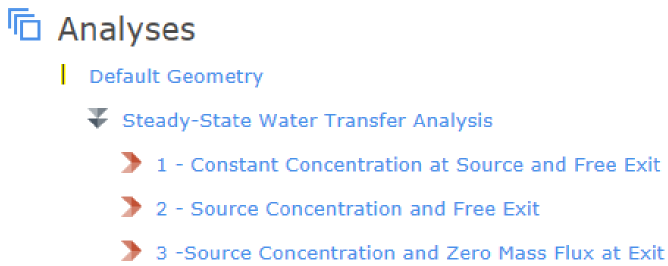

Figure 2. Analyses tree for the Project file.

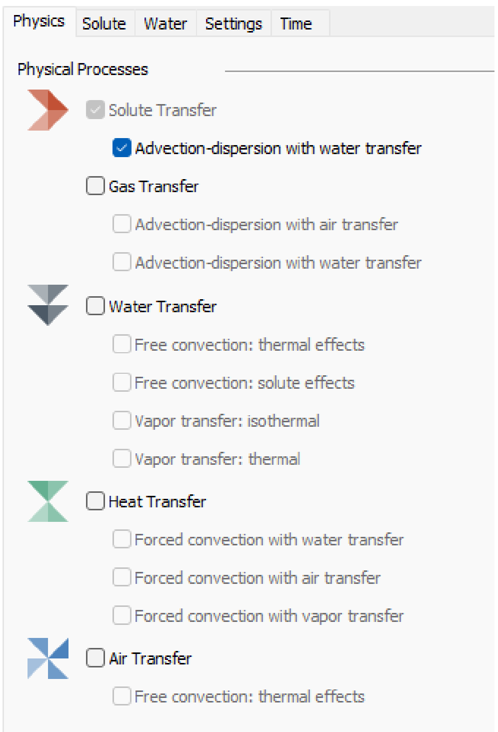

Figure 3. Physics tab for the solute transfer analyses.

The hydraulic properties are characterized using the Saturated-Only material model. The saturated hydraulic conductivity and volumetric water content are assumed equal to 0.5 m/sec and 0.5, respectively. Constant total head boundary conditions of 5 m and 1 m are specified on the left and right-hand sides of the domain, respectively. This leads to a total head loss of 4 m over the 40 m-long horizontal column, making the hydraulic gradient equal to 0.1 m/m, the water flux (or Darcy flux) equal to 0.05 m³/s/m², and the interstitial velocity ($v = q/\theta_w$) equal to 0.1 m/s.

The transport properties include a negligible bulk diffusion coefficient and a dispersivity of 4 m, which makes the coefficient of hydrodynamic dispersion equal to mechanical dispersion, such that $D = D' = \alpha v =$ 0.4 m²/s. Decay and adsorption are not included in the analyses and the material is activated with a concentration of 0 Mg/m³.

In Case 1, a constant concentration of 1 Mg/m³ is specified on the left-hand side boundary while a solute free exit mass flux boundary condition allows mass to leave the domain via advection on the right-hand side of the domain. For the remaining two cases, a source boundary condition (qC) with a fluid concentration of 1 Mg/m³ is applied to the left-hand side boundary. In so doing, the concentration at the boundary depends on both the water flux and fluid concentration. This condition represents a contaminated body of water acting as a source to the soil. Case 2 uses a solute free exit mass flux boundary condition on the right-hand boundary for comparison with Case 1. Case 3 uses a zero-mass flux, which implies that mass cannot leave the domain. This type of boundary condition is equivalent to an unspecified boundary condition when using the divergence form of the contaminant transport equation.

Results and Discussion

Figure 4 presents the concentration distribution at each time step for Case 1. The concentration at the left boundary was specified as a constant concentration, so the value is constant at 1 Mg/m^3 throughout the duration of the analysis. Recall that a free exit mass flux boundary condition is applied on the right side. As a result, mass is allowed to leave the domain via advection.

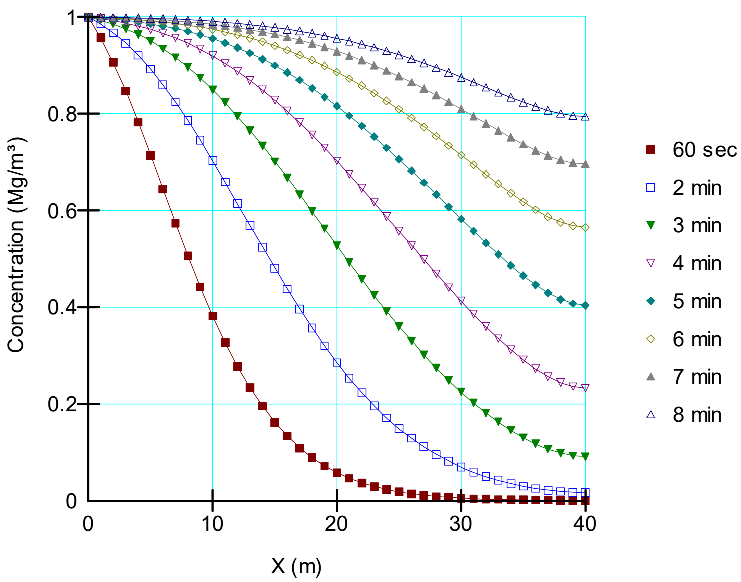

Figure 4. Case 1 – Concentration profiles.

Figure 5 shows the concentration distributions for Case 2 in which a source boundary condition with a fluid concentration of 1 Mg/m^3 is applied to the left-hand side of the domain. In this case, mass enters the domain at a flux equal to the product of water flux and concentration (qC) while the mass flux immediately inside the domain occurs by both advection (qC) and dispersion ($\theta_w DdC/dx$) due to groundwater flow and concentration gradients. The concentration at the boundary is less than 1.0 Mg/m^3 until the concentration gradient approaches zero, at which point the advection mass flux at the boundary becomes equal to the mass flux inside the domain. After some time, around 8 minutes, the concentration gradient approaches zero and the contours become perpendicular to the left-hand side boundary.

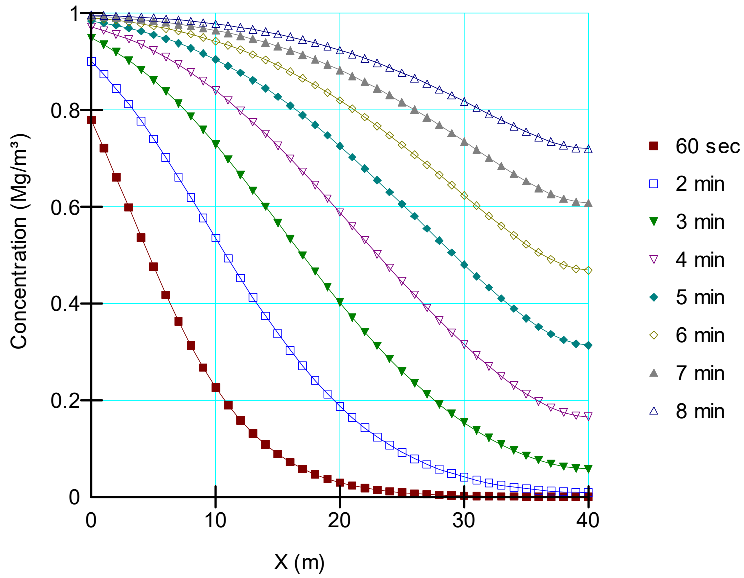

Figure 5. Case 2 – Concentration profiles.

Figure 6 compares the numerical solution (Case 2) to the closed-form solution for a semi-infinite medium with a source boundary condition. The differences are the result of the free exit boundary condition only allowing mass to leave by advection. The lack of dispersion through the right-hand side boundary produces a zero-gradient condition that propagates upstream from the boundary. The extent of the propagation increases with decreasing hydraulic gradient, and more specifically, as the dispersive component increases relative to the advective component. In some cases, the issue can be avoided or mitigated by moving the far-field boundary further from the source.

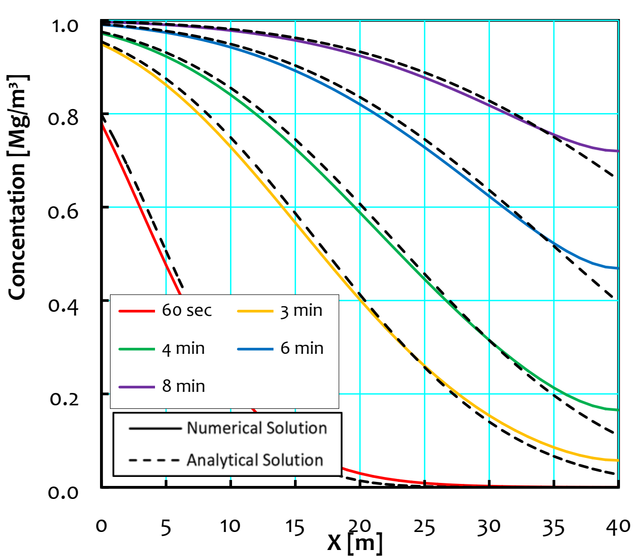

Figure 6. Comparison of the analytical solution for a semi-infinite domain to the numerical solution for a finite domain with a solute free exit mass flux boundary condition.

Figure 7 presents the concentration distributions for Case 3 in which a zero-mass flux boundary condition is applied to the right-hand side of the domain. In this case, the mass accumulates at the boundary where the concentration ultimately becomes larger than the source concentration. The application of a zero-mass flux boundary condition is redundant, and the results are identical to those found when no solute boundary condition is applied. Again, the divergence of both the advective and dispersive mass flux is implicitly zero if a boundary condition has not been applied.

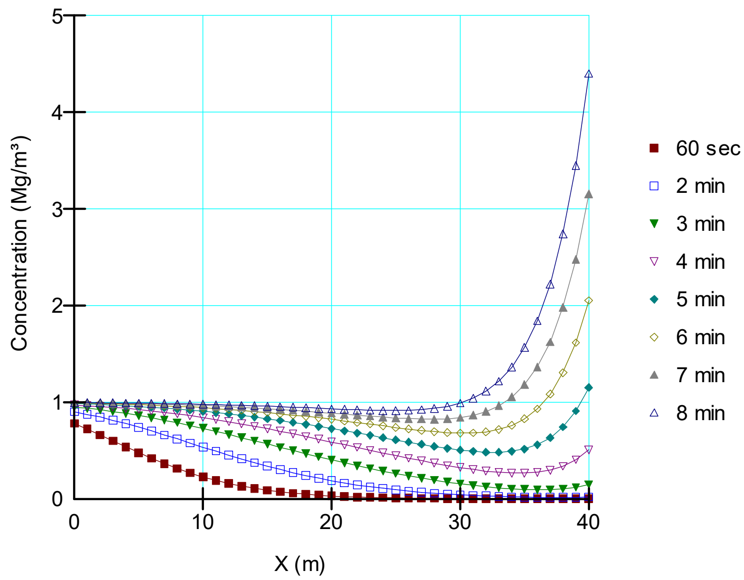

Figure 7. Case 3 – Concentration profiles.

Summary and Conclusions

The main objective of this example was to compare results obtained using two options for the source boundary and two options for the exit boundary. The constant concentration boundary condition was found to force the concentration at the source to remain constant while the source boundary condition allowed the concentration at the source to increase with time until it reached the specified concentration. The zero-mass flux boundary condition was found to lead to an increase in concentration at the exit boundary as it prevented the solute from leaving the domain by both dispersion and advection. The boundary condition was referred to as redundant given that the natural boundary condition for the divergence form of the solute transfer equation is zero divergence of the dispersive and advective mass rate. The solute free exit mass flux boundary condition (not to be confused with Frind's free exit boundary condition) was found to allow mass to leave the domain via advection.

The last objective of this example was to compare the numerical solution of the source concentration and solute free exit mass flux boundary condition with the closed-form solution of the advection-dispersion equation for a one-dimensional semi-infinite medium with a source boundary condition. The results generally compared well with the closed-form solution, but some differences were noted in the vicinity of the boundary where the solute exited the domain via advection and the lack of dispersion produced a zero-gradient condition. This could have been resolved by moving the boundary to the far field.

References

Frind, E.O., 1988. Solution of the advection-dispersion equation with free exit boundary. Numerical Methods for Partial Differential Equations, 4(4): 301-313.