GeoStudio Example File
CTRAN Tutorial

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Introduction

The objective of this analysis is to demonstrate how CTRAN/W can be used to model solute transport by advection and dispersion. The analysis involves establishing the groundwater flow conditions and defining the appropriate material properties and boundary conditions. It also highlights the importance of selecting the correct solute boundary condition at the groundwater discharge location.

Background

A solute will migrate through the soil due to three processes: diffusion, dispersion and advection. The first two processes, diffusion and dispersion, occur in response to concentration gradients while advection occurs as the solute is carried along by the flowing water. The divergence form of the one-dimensional advection-dispersion equation for a homogeneous and isotropic material reads as follows (de Marsily, 1986):

$$\frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x} - Cv_x\right] = \frac{\partial C}{\partial t}$$

Equation 1

where D is the coefficient of hydrodynamic dispersion, C is the concentration, $v_x = q_x/\theta_w$ is the average linear velocity in the x-direction, q_x is the Darcy flux in the x-direction, θ_w is the volumetric water content, and t is time. The first component of the term on the left-hand side of the equation represents the dispersive transport while the second component represents advection via flowing water. The dispersive term incorporates diffusion and the scale-dependent mechanical mixing caused by local variations in fluid velocity. This equation emphasizes the importance of establishing the water flow conditions to accurately simulate transport processes.

Numerical Simulation

Figure 1 shows the two-dimensional domain in which a pond lies on an upland silty plateau near a lowland floodplain. The volumetric water content function, shown in Figure 2, is estimated using the sample silt material with an assumed porosity of 0.35. The hydraulic conductivity function, shown in Figure 3, is estimated using van Genuchten's model and an assumed saturated hydraulic conductivity of 0.01 m/day (1.16×10^{-7} m/s).

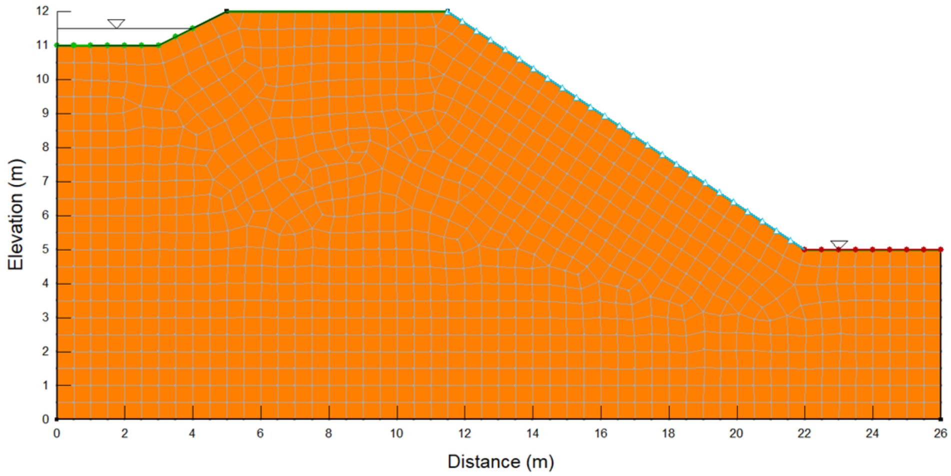

Figure 1. Problem configuration.

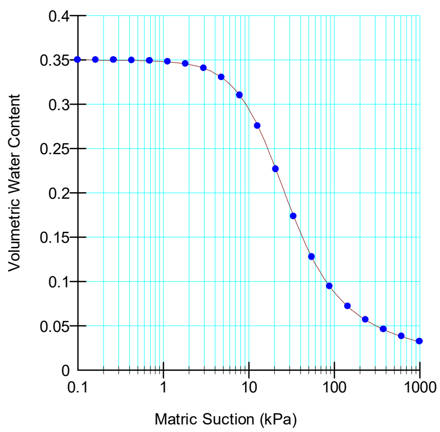

Figure 2. Volumetric water content function of the sample silt material.

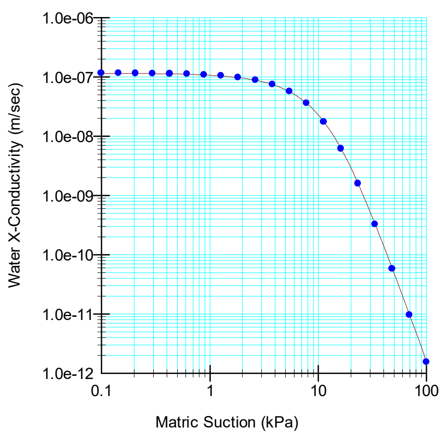

Figure 3. Hydraulic conductivity function of the sample silt material.

The pond is modeled using a total head boundary condition of 11.5 m while a potential seepage face review boundary condition is applied to the entire slope face and a zero-pressure boundary condition is applied to the soil surface along the lowland floodplain on the right-hand side of the domain. As shown in Figure 4, the results of the steady-state water transfer analysis serve as the parent for three contaminant transport analyses.

Figure 4. Analysis Tree for the GeoStudio project.

Figure 5 shows the physical settings used to model contaminant leaching from the pond. Although diffusion is a default physical process in a solute transfer analysis, advection and dispersion must be toggled on as additional processes. As shown in Figure 6, the contaminant transport analyses must explicitly state that the water transfer results are taken from the parent analysis.

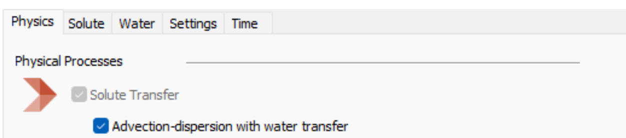

Figure 5. Physics tab with advection-dispersion process activated.

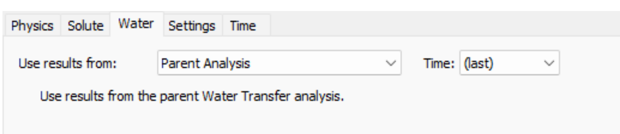

Figure 6. Water tab with water transfer results taken from the parent steady-state analysis.

A constant concentration boundary condition of 1000 g/m³ is used to represent the contaminant in the pond. Figure 7 shows the solute material property window in which the activation (or initial) concentration is set equal to 0 g/m³. The material property window also contains the longitudinal and transverse dispersivity, which are arbitrarily set equal to two and one meters, respectively. These parameters depict a measure of the mixing and spreading that will occur as the solute moves along with the flowing water. Decay and adsorption were not included in the example.

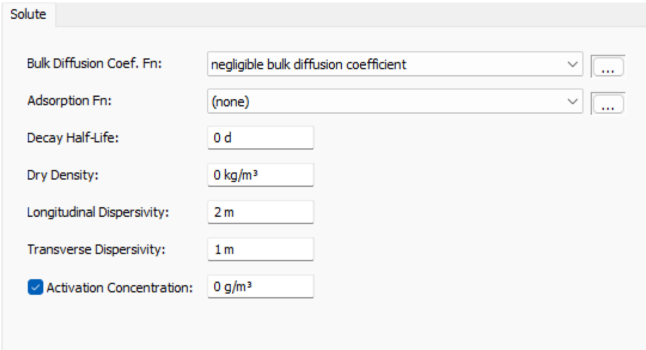

Figure 7. Solute material properties for the advection-dispersion analysis.

The discharge location is modeled using three different boundary conditions: (1) Unspecified (no boundary condition is applied), (2) A zero total mass flux boundary condition, and (3) A solute free exit mass flux boundary condition, which allows mass to leave the domain via advection. The first contaminant transport analysis includes tracking of three particles defined near the base of the pond. The location of these particles is solely based on the groundwater velocity, which represents advective transport.

The duration of the transient analyses is set equal to 2750 days (approximately 7.5 years) with 55 linearly distributed timesteps. The approximate global element mesh size is set equal to 0.5 m for the entire domain.

Results and Discussion

Figure 8 presents the total head contours (equipotential lines), water flux vectors, and phreatic surface for the steady-state water transfer analysis. A seepage face has developed near the toe of the slope. The water flux within the saturated zone and along the primary pathway for flow is around 2.5×10^{-8} m/s, which translates into a velocity $v = q/\theta_w =$ 7.14×10^{-8} m/sec.

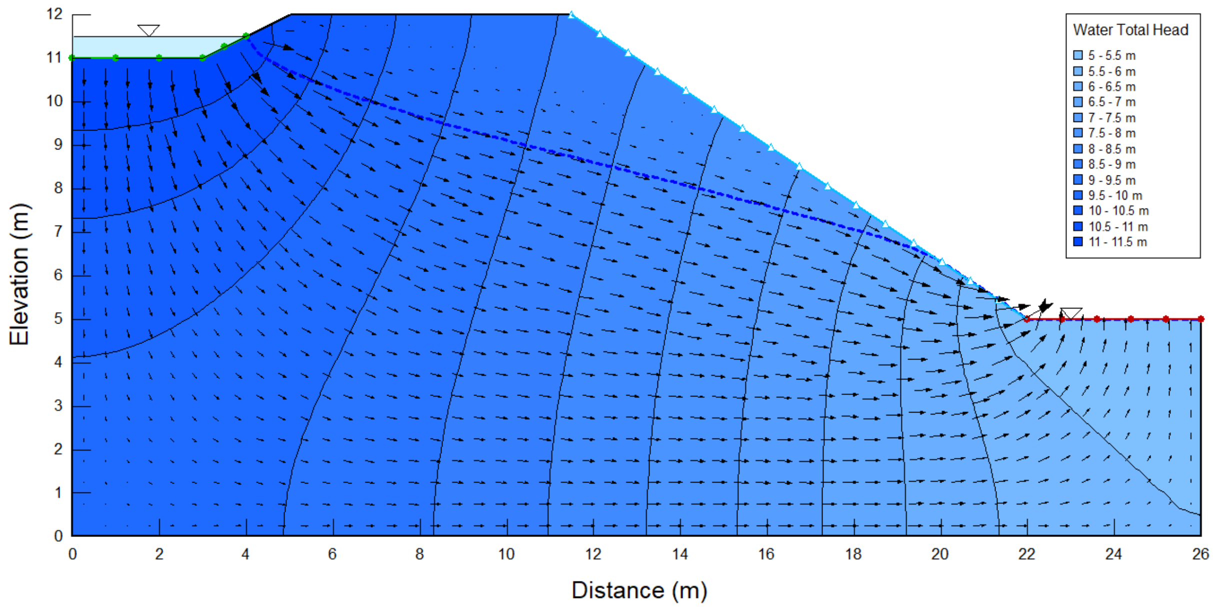

Figure 8. Resulting flow regime for the steady-state water transfer analysis.

Figure 9 presents the concentration contours and solute mass flux vectors at the final timestep for Case 1. The solute mass flux vectors (in red) confirm that transport is governed by advection given that the vectors are mostly parallel to the water flux vectors (in black). The concentration diminishes towards the crest of the slope where the water has essentially stagnated. Recall that a solute boundary condition was not applied to the ground surface in this case. The second-type boundary condition, also termed the natural boundary condition, is total mass rate equal to zero. Mass cannot leave the domain by dispersion or advection if water is crossing the domain boundary. As a result, the solute accumulates near the toe of the slope as the solute-free water leaves the domain. The accumulation of the solute eventually leads to concentrations that exceed the source value. In this and subsequent cases, the top-most particle travels approximately 20 m at an average velocity of 8.4×10^{-8} m/sec, which is in-keeping with the approximate value calculated above. The lower-most particle travels 12.5 m over the same duration. A shorter travel distance is expected as the average water flux decreases towards the lower-left-hand-side of the domain. The spreading of the contaminant past the location of the particles is a manifestation of dispersive transport.

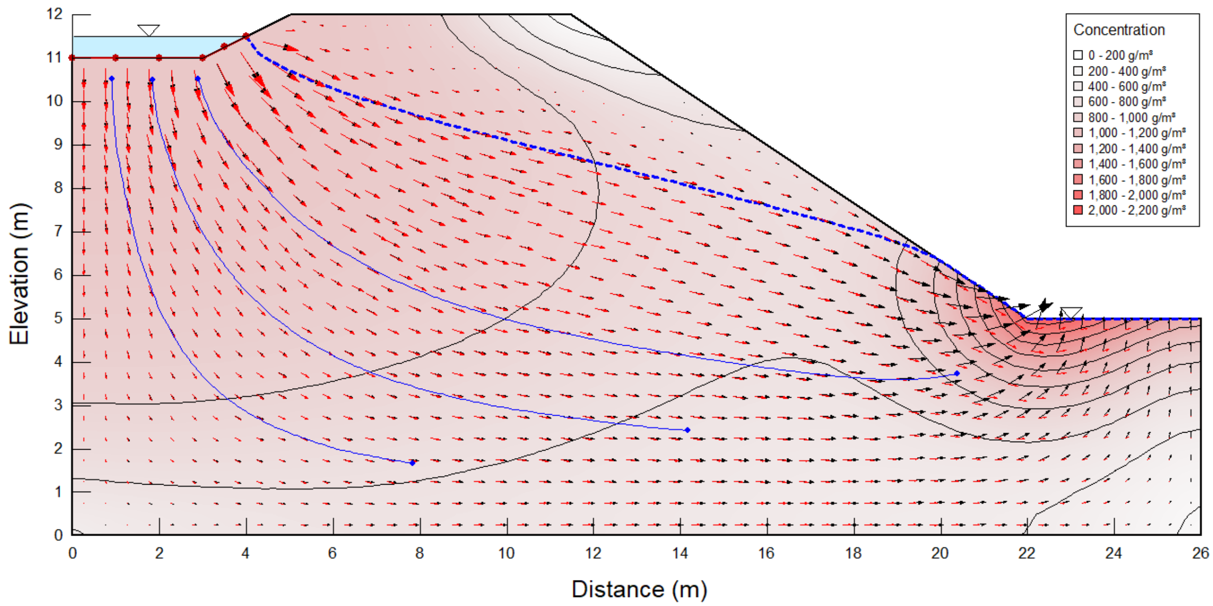

Figure 9. Case 1 – Concentration contours.

Figure 10 shows the concentration contours and solute mass flux vectors for Case 2 in which a zero total mass flux boundary condition is applied to the ground surface on the right-hand side of the domain. As expected, the boundary condition is redundant, and the results are identical to those found when no solute boundary condition is applied.

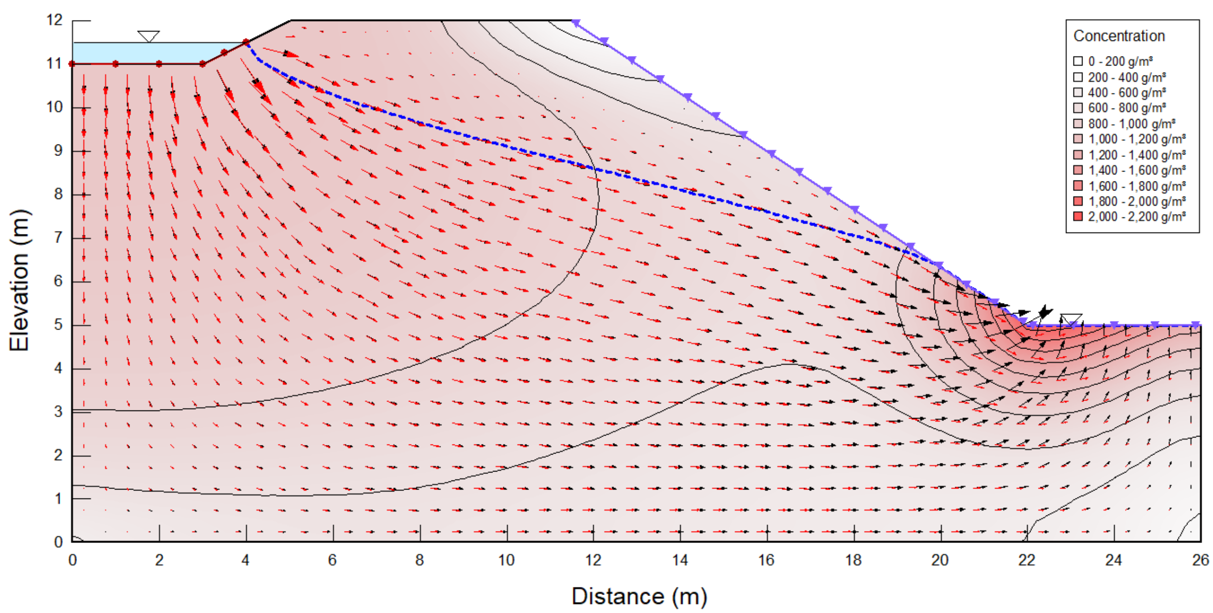

Figure 10. Case 2 – Concentration contours.

Figure 11 shows the concentration contours and solute mass flux vectors for Case 3 in which the solute free exit mass flux boundary condition allows mass to leave the domain by advection. The concentration slowly increases with time, but never exceeds the source concentration. The discharge mass rate, shown in Figure 12, slowly increases with time as mass starts to leave the domain after 1000 days.

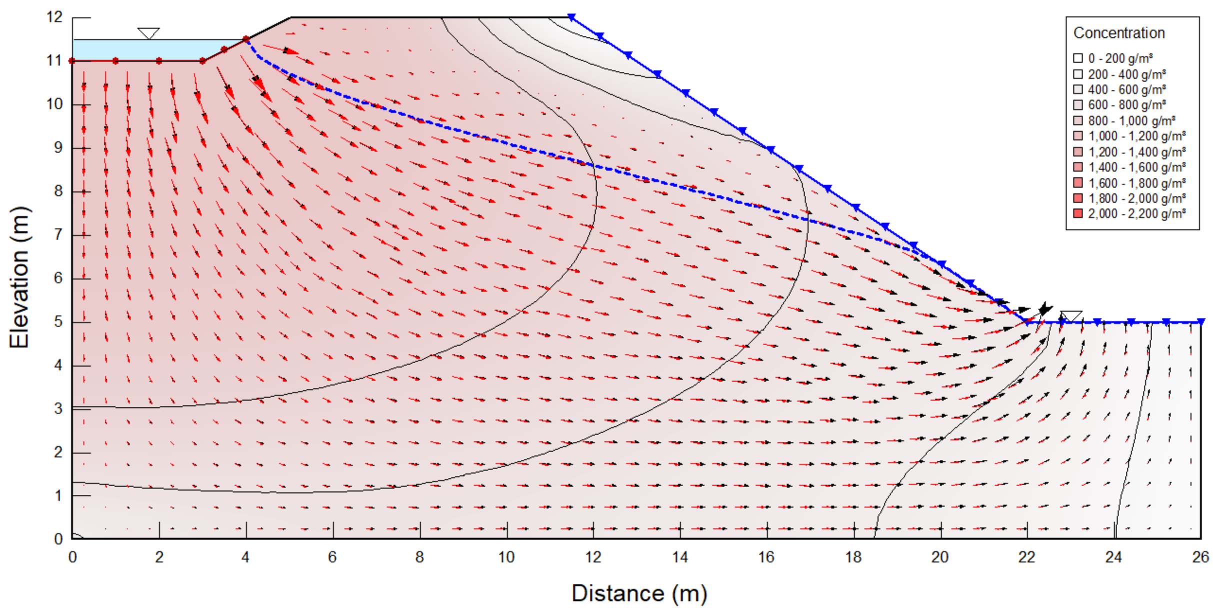

Figure 11. Case 3 – Concentration contours for case 3.

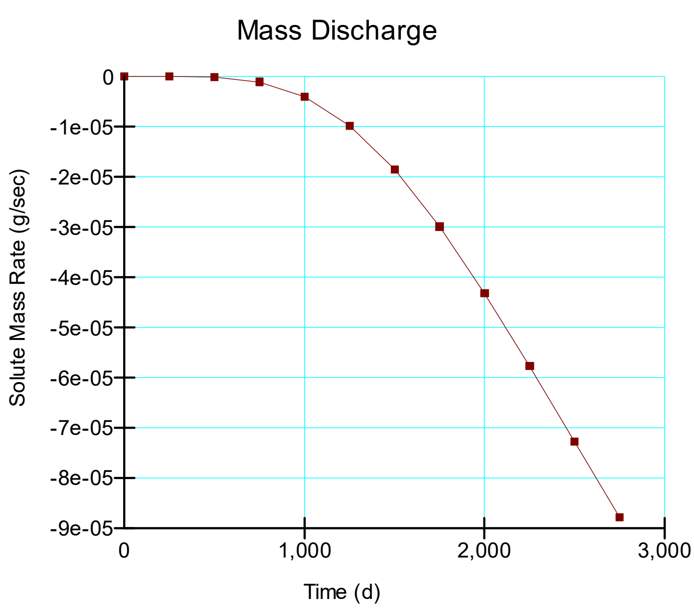

Figure 12. Case 3 – Mass discharge along the ground surface.

Summary and Conclusions

This example focused on contaminant transport via advection and dispersion from a pond to a downslope location. The results highlighted the effect of various solute boundary conditions at the water discharge location. Leaving the discharge boundary unspecified forced the total solute mass flux to zero. This resulted in an accumulation of solute and concentrations that exceeded the source value near the boundary as the solute-free water exited the domain. Identical results were found when applying a zero total mass flux boundary condition. Applying a solute free exit mass flux boundary allowed solute to leave the domain via advection. This resulted in mass discharge and a slight increase in concentration that never exceeded the source value near the boundary. The example also highlighted the mixing effect of dispersion that occurs as the concentration spreads beyond the distance that a particle would travel by advection-alone.

References

de Marsily, G. 1986. Quantitative hydrogeology: Groundwater hydrology for engineers. Academic Press Inc., Orlando, Florida.