CTRAN Tutorial

GEO-SLOPE International Ltd. | www.geo-slope.com

1200, 700 - 6th Ave SW, Calgary, AB, Canada T2P 0T8
Main: +1 403 269 2002 | Fax: +1 888 463 2239

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 two processes: diffusion and advection. Diffusion occurs in response to concentration gradients, while advection occurs as the solute is carried along by the flowing water. The one-dimensional advection-dispersion equation for a homogeneous, isotropic material is defined as:

$$D\frac{\partial^2 C}{\partial x^2} - v_x\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \qquad \text{Equation 1}$$

where D is the coefficient of hydrodynamic dispersion, C is the concentration, v_x is the average linear velocity in the x-direction, which is equal to the Darcy flux (q) divided by the effective porosity (n_e), and t is time (Fetter, 1993). The first term on the left represents the dispersive transport and the second term represents advection via flowing water. The dispersive term incorporates diffusion and the scale-dependent mechanical mixing caused by local variations in velocity. This equation emphasizes the importance of establishing the water flow conditions to accurately simulate transport processes.

Numerical Simulation

The two-dimensional model domain is shown in Figure 1. There are four analyses in the file, with the steady-state water transfer analysis acting as the Parent for all three transient contaminant transport analyses (Figure 2). A pond is located on the upland of a slope and is modeled using a total head boundary condition of 11.5 m. The potential seepage face boundary condition has been applied to the entire slope face, with a zero pressure boundary condition applied to the soil surface along the lowland on the right.

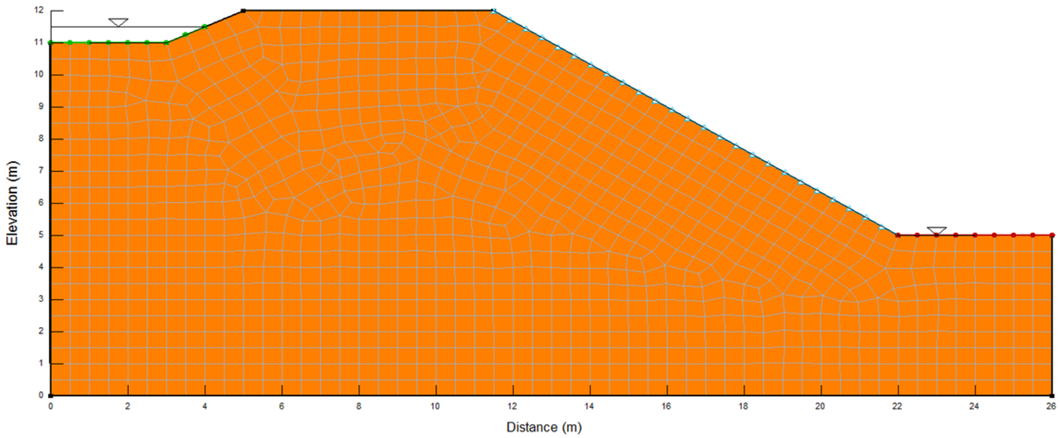


Figure 1. Problem configuration.

Analyses

Steady-state Seepage

1 - Exit Boundary Unspecified

2 - Zero Total Flux at Exit Boundary

3 - Exit Review Boundary

Figure 2. Analysis Tree for the GeoStudio project.

The sample function for silt was used to estimate the volumetric water content and hydraulic conductivity function for a saturated-unsaturated material model. The porosity and saturated hydraulic conductivity were assumed to be 0.35 and 0.01 m/day (1.16×10^{-7} m/sec), respectively (Figure 3 and Figure 4).

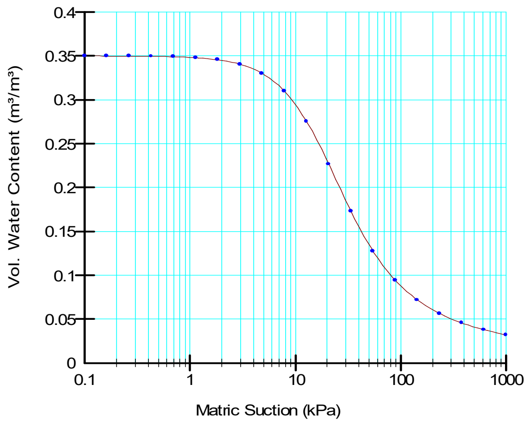


Figure 3. Volumetric water content function for a silt sample material.

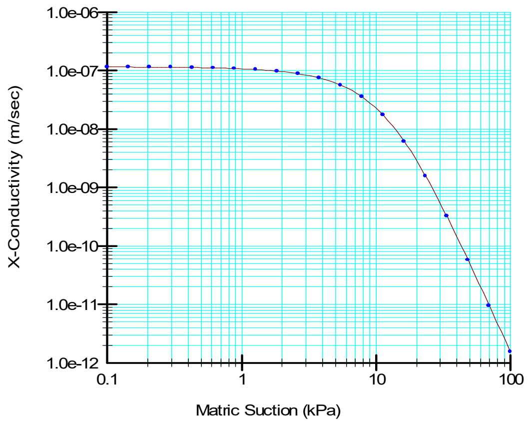
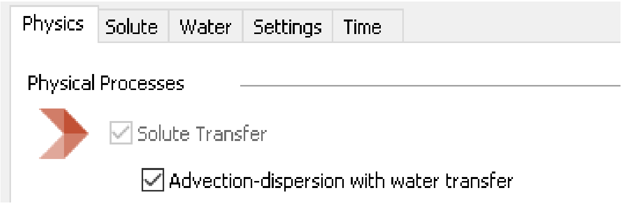


Figure 4. Hydraulic conductivity function for a silt sample material.

The solute transport analyses are configured to simulate contaminant leaching from the pond. The default physical process for a CTRAN/W analysis is diffusion. In order to simulate advection and dispersion, the "Advection-dispersion with water transfer" option is activated on the physics tab (Figure 5). The water transfer results are defined using the parent steady-state water transfer analysis (Figure 6).

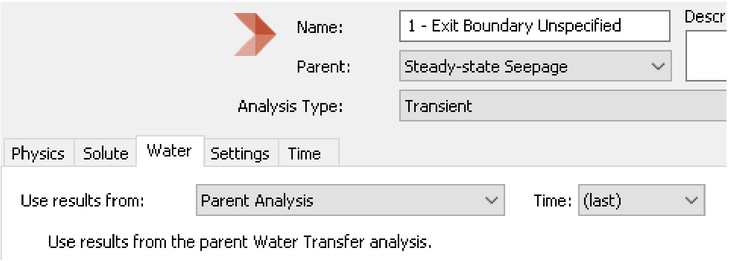


Physical Processes

☑ Solute Transfer

☑ Advection-dispersion with water transfer

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


Name: 1 - Exit Boundary Unspecified

Parent: Steady-state Seepage

Analysis Type: Transient

Use results from: Parent Analysis

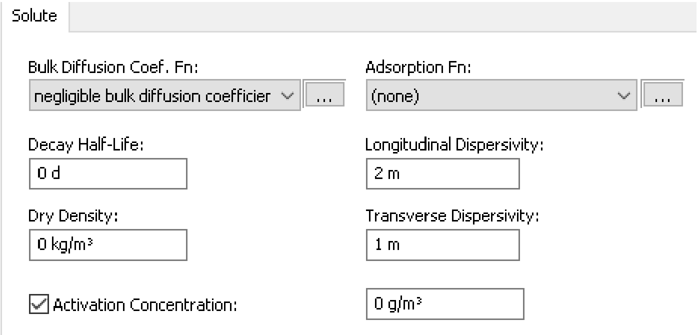
Time: (last)

Use results from the parent Water Transfer analysis.

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

A constant concentration boundary condition of 1,000 g/m³ is used to represent contaminant in the pond. The initial concentration of the soil is defined as 0 g/m³ using the activation concentration option in the material property window (Figure 7). A different boundary condition was used to model the discharge location in the three cases. In Case 1, the exit boundary is unspecified (no boundary condition applied). A zero total mass flux and free exit mass flux boundary condition were used in Cases 2 and 3, respectively. A free exit condition allows mass to leave the domain via advection and dispersion if the concentration exceeds 0 g/m³.

The material inputs for an Advection-Dispersion analysis requires a definition for dispersivity (Figure 7). In this case, the longitudinal dispersivity is arbitrarily defined as 2 m and the transverse dispersivity is defined as 1 m. These parameters depict a measure of the mixing that will occur as the solute moves along with the flowing water. Decay and adsorption were not included in this example.


Bulk Diffusion Coef. Fn: negligible bulk diffusion coefficier

Adsorption Fn: (none)

Decay Half-Life: 0 d

Longitudinal Dispersivity: 2 m

Dry Density: 0 kg/m³

Transverse Dispersivity: 1 m

☑ Activation Concentration: 0 g/m³

Figure 7. Material properties for an Advection-Dispersion analysis.

Particle tracking was also conducted by defining particles near the base of the pond in Case 1. CTRAN/W tracks the location of these particles based solely on the groundwater velocity, which represents transport by advection-only.

The duration of the transient analyses were set to approximately 7.5 years with 55 time steps increasing linearly with time increments of 50 days each. The global element mesh size was set to 0.5 m for the entire domain.

Results and Discussion

The simulated total head contours (equipotential lines), water flux vectors, and phreatic surface for the steady-state flow regime are shown in Figure 8. It can be seen that 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 2.5e-8 m/s. The calculated velocity for a saturated porosity of 0.35 is therefore 7.14e-8 m/sec.

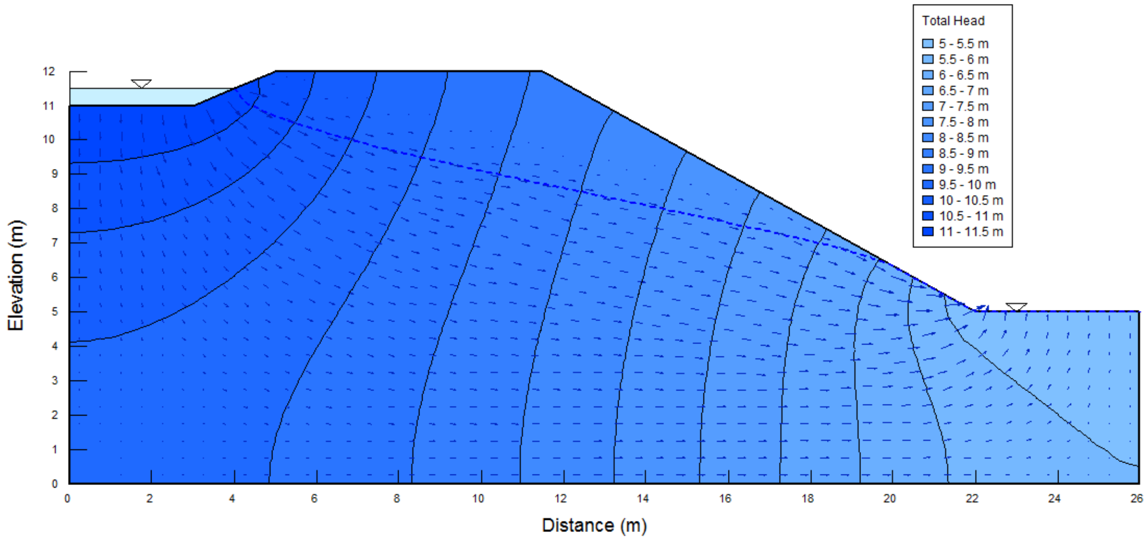


Figure 8. Resulting flow regime for the steady-state water transfer analysis.

Figure 9 presents the simulated concentration distribution for Case 1 after 7.5 years, along with the location of the particles. Figure 10 presents the mass discharge rate along the ground surface. The solute reaches the ground surface at about Day 1000. The solute mass flux vectors confirm that transport is governed by the advection because the vectors are nearly parallel to the water flux vectors. 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 Case 1. The 2^{nd} type boundary condition, also termed the natural boundary condition, is dispersive mass rate equal to zero. Mass can leave the domain by advection if water is crossing the domain boundary but, the natural boundary condition requires that the concentration gradient normal to the surface be zero. It is for this reason that the concentration contours are perpendicular to the exit boundary (Figure 9). Similarly, the contours are perpendicular to the boundaries along the other edges and the total mass flux is zero because water is not crossing boundaries.

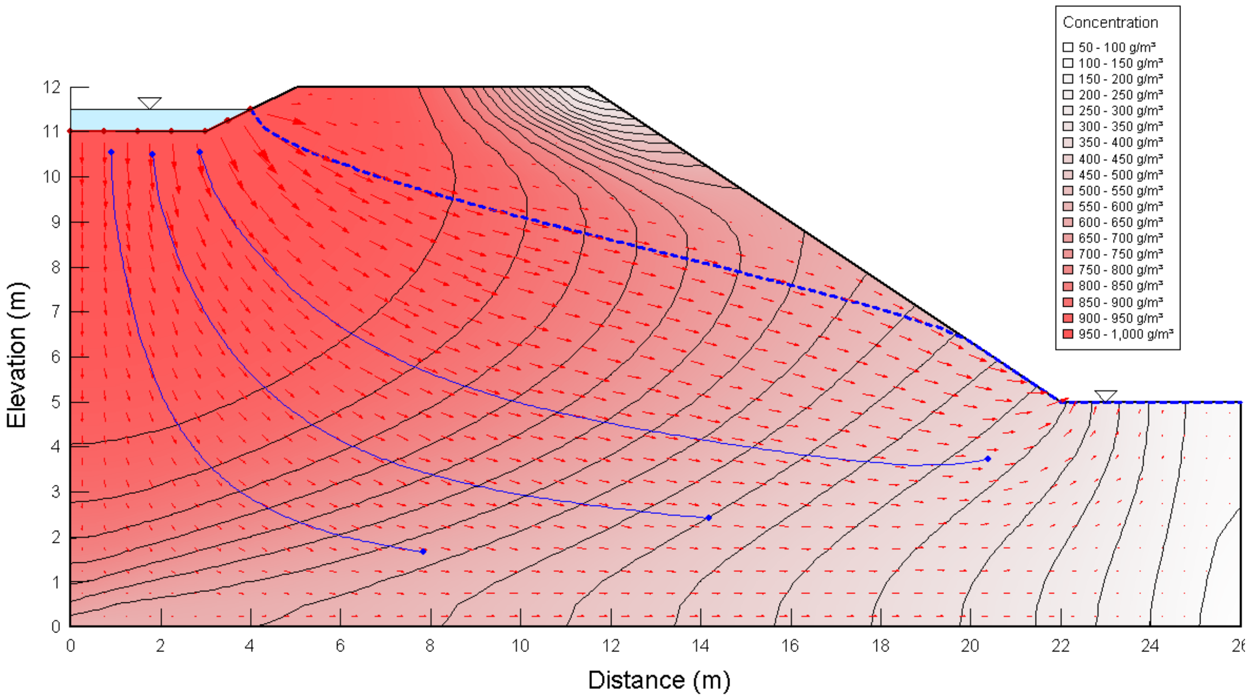


Figure 9. Concentration distribution after an approximate duration of 7.5 years.

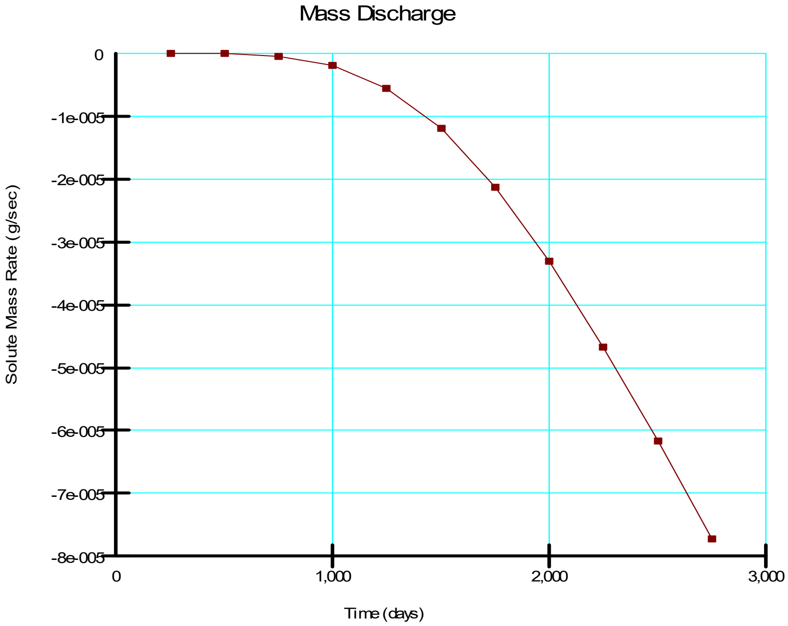


Figure 10. Mass discharge along the ground surface.

The top-most particle has travelled approximately 20 m at an average velocity of 8.4e-8 m/sec, which is in-keeping with the approximate value calculated above. The lower-most particle has travelled 12.5 m over the same duration. The smaller travel distance is expected as the average water flux decreases towards the lower-left area of the domain. The spreading of the contaminant past the location of the particles is a manifestation of dispersive transport.

Figure 11 and Figure 12 present the concentration contours for Case 2 and Case 3. In Case 2, mass is accumulating near the toe of the slope as water leaves the domain, but the solute remains due to the zero total mass rate boundary condition. In turn, the concentration begins to exceed the source concentration. The concentration contours for Case 3 look similar to Case 1 as the free exit mass flux boundary condition allows mass to leave the domain via advection and dispersion. The contours near the toe are no longer perpendicular for Case 3. Finally, it is noted that the mass discharge reported on the graph for Case 2 is not zero despite the specified zero total flux boundary condition. This occurs because reassembly of the nodal mass rates post-solve yields a value if the water rate and concentration are non-zero.

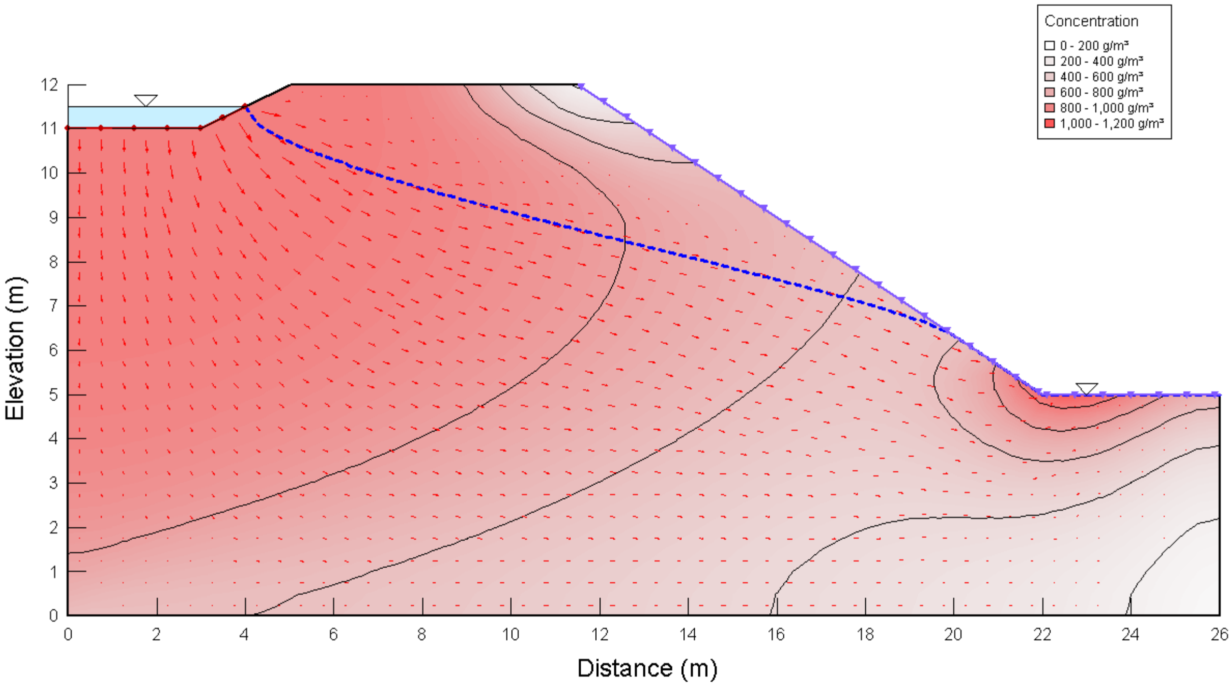


Figure 11. Concentration contours for Case 2.

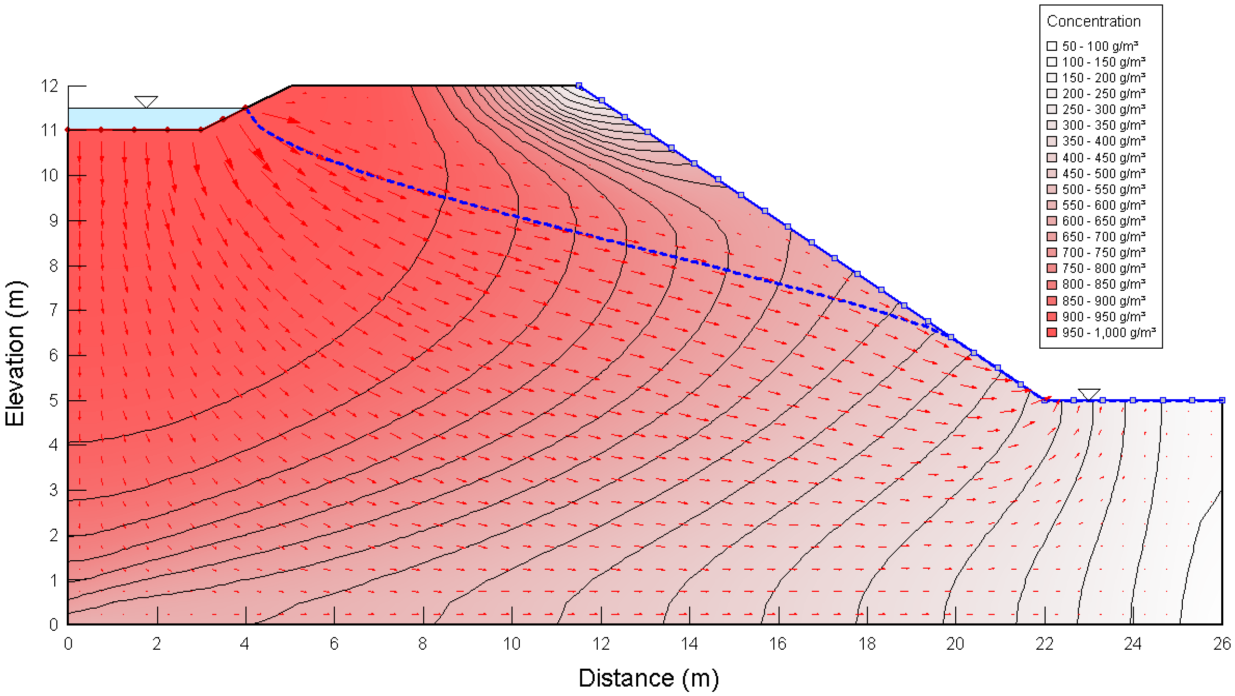


Figure 12. Concentration contours for case 3.

Summary and Conclusions

A numerical analysis of contaminant transport via advection and dispersion from a pond to a downslope location was conducted in this example. The results highlight the effect of various solute boundary conditions at the water discharge location. Leaving the discharge boundary unspecified implies that dispersive solute flux is zero, while mass can still leave the domain via advection. This results in concentration contours that are perpendicular to the water discharge boundary. In contrast, applying a total mass flux equal to zero boundary forces both the advection and dispersive flux to zero. Mass accumulated near the boundary and the concentration exceeded the source value. A free-exit mass flux boundary condition allows mass to exit via dispersion and advection. This example also highlights the spreading effect of dispersion, as the concentration spreads beyond the distance that a particle would travel by advection-alone.

References

Fetter, C.W. 1993. Contaminant hydrogeology. Macmillan Publishing Company, New York, NY. pp. 52-54.