SOFTWARE VALIDATION TEST PLAN AND REPORT FOR HYDRUS VERSION BETA.03

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1 SOFTWARE VALIDATION TEST PLAN AND REPORT FOR HYDRUS VERSION BETA.03

This software validation test plan and report pertains to HYDRUS Version Beta.03 (Simunek, et al., 2006a). Henceforth, this version of the program will simply be referred to as HYDRUS. HYDRUS was originally developed by Simunek, et al. (1999) as HYDRUS-2D to simulate the movement of water, heat, and multiple reactive solutes in variably saturated porous media in two dimensions. HYDRUS-2D is widely used by academic researchers and geoscientists to simulate flow and transport processes in partially saturated porous media. The beta version of HYDRUS is the only version commercially available and is an extension of the modeling procedures used in HYDRUS-2D to three dimensions. HYDRUS solves the flow and transport equations using the finite element method. The flow equation is formulated based on the Richards' equation. The solute transport equation and heat transport equation are based on the standard advective-dispersion equation using a Fickian model for dispersion. The same is true for the heat transport equation. Solute concentrations in the pore water are assumed to be sufficiently low that the water density is constant; thus the computed water flux is not affected by density variations or osmotic effects, and the flow equations are not dependent on the solute transport equations. As with solute transport, the heat transport is dependent on the water fluxes. Temperature affects the water flux only by modifying soil hydraulic properties; thus the model does not include thermal diffusion of water. Because the temperature distribution affects the hydraulic properties of the medium, the water flow and heat transport equations are solved iteratively. Thermal effects are not included in the transport equations.

2 SCOPE OF VALIDATION

HYDRUS has been used extensively for various applications in the fields of soil science, unsaturated zone hydrology, and environmental assessments and has been subject to previous validation exercises using field and laboratory data (e.g., Simunek, et al., 1999; Simunek, et al., 2006b; Nolan, et al., 2005). HYDRUS includes a wide range of features, not all of which are addressed in this validation exercise. For example, the program provides several models for describing hydraulic properties under partially saturated conditions, but only the van Genuchten and Brooks-Corey models are considered here. HYDRUS also includes options for simulating flow and transport in dual porosity media, but only the single porosity features are addressed in this validation. In addition, HYDRUS includes a number of options for simulating sorption, phase partitioning, and decay. Only the basic transport features are considered in this validation. Finally, HYDRUS includes capabilities for hydraulic parameter estimation by numerical inversion. Because many of the HYDRUS features have been tested elsewhere, the scope of this validation will be limited to (i) comparing HYDRUS results to an analytic solution for vertical, steady-state flow in a partially saturated soil column; (ii) comparing HYDRUS results to an independent application of HYDRUS-2D for a transient flow problem; and (iii) comparing HYDRUS simulations of mass transport with an analytic solution.

Specific validation simulations include

- Simulation of steady-state pressure head distribution in a soil column with steady evaporation (Salvucci, 1993)

- Simulation of transient two-dimensional soil water distribution near a land mine (Rhebergen, et al., 2002)

- Simulation of one-dimensional transport of a radioactive substance in a semi-infinite column (Javandel, et al., 1984)

The features of HYDRUS not specifically considered in this validation should be tested as specific modeling needs arise.

3 REFERENCES

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4 ENVIRONMENT

4.1 Software

The HYDRUS Version Beta.03 software was obtained from PC-Progress, Prague, Czech Republic. The program was installed on a personal computer with Microsoft® Windows® 2000 Professional operating system. Postprocessing of output was performed with Microsoft® Excel® 2002, SP-2.

4.2 Hardware

The personal computer on which the HYDRUS simulations were performed (MAGE) had an Intel® Pentium® 4 processor.

5 PREREQUISITES

None.

6 ASSUMPTIONS AND CONSTRAINTS

The numerical procedures for simulating water flow under partially saturated conditions are based on the Richards' equation, which assumes that water flow is not affected by the movement of soil gas; thus use of this model may not be appropriate for cases with strong coupling between water and gas flow. The constitutive equations used in HYDRUS to represent soil hydraulic properties are based on empirical relationships derived for porous media and may not be applicable for cases of fracture-dominated flow.

The numerical procedures used to simulate mass transport are based on classical formulations of the advection-dispersion equation and assume a Fickian model of hydrodynamic dispersion. The numerical procedures used to simulate chain decay reactions were not validated for this report.

The numerical procedures used to simulate heat transport are based on a classical formulation of the advection-conduction equation and do not consider the effects of hydrodynamic dispersion. The heat transport equation also does not consider the effects of heat transport by water vapor movement. The numerical procedures used to simulate heat transport were not validated for this report.

7 TEST CASES

7.1 Test Case 1: Steady-State Tension Head Distribution in Vertical Column

Test Case 1 compares HYDRUS results with an approximate analytic solution by Salvucci (1993) for the tension head distribution in a vertical, homogeneous soil column with constant evaporation at its upper surface. Salvucci's solution in terms of elevation and tension head is

$$\frac{z}{\psi_1} = \frac{1}{1+q'}\left[\frac{q'}{1+q'} + \left(\frac{\psi}{\psi_1}\right)^{-n}\right]^{-1/n} \tag{1}$$

where

z	—	vertical coordinate [cm]
ψ_1	—	bubbling head [cm]
q'	—	surface flux q [cm/s] divided by the saturated hydraulic conductivity K_s [cm/s]
ψ	—	tension head at z [cm]
n	—	empirical coefficient used to relate the hydraulic conductivity to the tension head [dimensionless]

Salvucci's solution assumes that the hydraulic conductivity is related to the tension head by

$$K(\psi) = \frac{K_s}{1+\left(\frac{\psi}{\psi_1}\right)^n} \tag{2}$$

where K_s is the saturated hydraulic conductivity. For the case of surface evaporation, the surface flux is taken as positive, and the lower boundary of the soil column is saturated [ψ (z = 0) = 0].

The HYDRUS simulation of this problem utilizes the finite element mesh shown in Figure 1. The mesh consists of two nodes horizontally and 20 nodes vertically. Even though this is a one-dimensional flow problem, HYDRUS requires using a two-dimensional mesh. The lower model boundary condition is a constant tension head set at zero. The upper boundary condition is constant flux equal to -1.58×10^{-6} cm/s [-6.22×10^{-7} in/s], which is equivalent to -50 cm/yr [-20 in/yr]. Simulations are performed using the default soil hydraulic properties for a clay loam and a sandy loam provided in HYDRUS. These properties are listed in Table 1. The soil hydraulic properties model used in the simulations was the Brooks-Corey model in which the hydraulic conductivity versus tension head relationship is given by Eq. (3)

$$K(\psi) = K_s\left(\frac{\psi_1}{\psi}\right)^{2+3m} \tag{3}$$

where m is an empirical coefficient. Although the hydraulic conductivity function given by Eq. (3) is not identical to that used by Salvucci [Eq. (2)], the two are approximately the same for relative dry conditions ($\psi >> \psi_1$) and n is related to m by

$$\frac{n-2}{3} = m \tag{4}$$

The initial condition for the HYDRUS simulations is to set the tension head to -100 cm [-39 in] throughout the model domain.

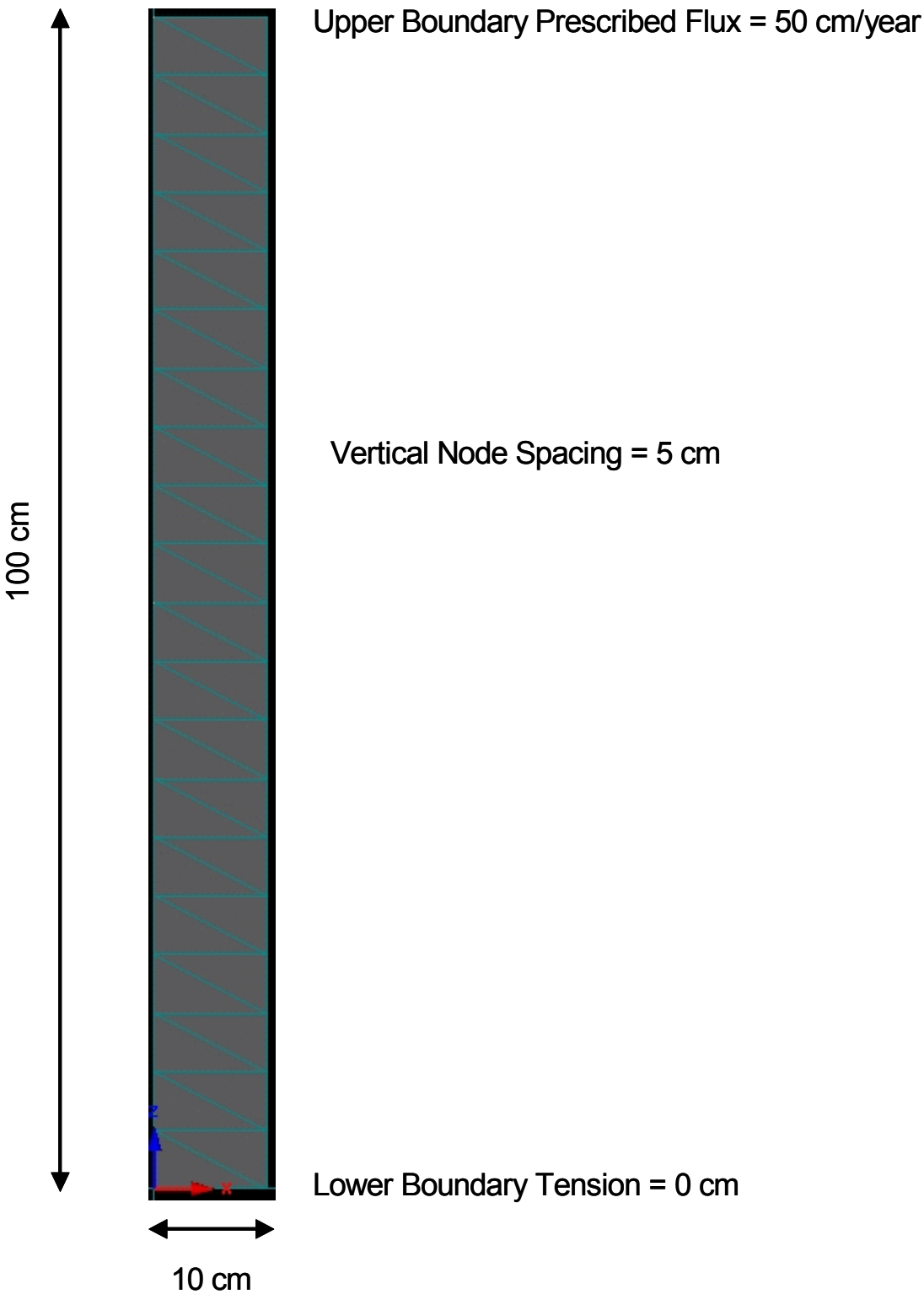

Figure 1. Finite Element Mesh Used for Test Case 1 [1 cm = 0.39 in]

Table 1. Hydraulic Properties Used in Test 1 Simulation				
Soil	**K_s (cm/s)***	**ψ_1 (cm)***	**Salvucci *n***	**Brooks-Corey *m***
Clay Loam	6.39×10^{-5}	25.9	2.582	0.194
Sandy Loam	7.19×10^{-4}	14.7	2.966	0.322
*1 cm = 0.39 in				

7.1.1 Input Files for Test Case 1

The HYDRUS input files for the clay loam simulation are contained in directory *H3D_1-dsalvucci clay loam*. The HYDRUS input files for the sandy loam simulation are contained in directory *H3D_1-dsalvucci sandy loam*. The Salvucci analytic solution is implemented in the spreadsheet *salvucci.xls*.

7.1.2 Test Procedure

1. Run the HYDRUS simulations for 8.64×10^5 seconds to establish quasi-steady-state conditions.

2. Export the finite element mesh and final tension heads from HYDRUS to ASCII text files (see the HYDRUS User Manual for explanation of this procedure). These files are named *MESHTRIA.TXT* and *H.TXT*, respectively.

3. Copy the coordinates of one vertical set of nodes to *salvucci.xls*. Copy the corresponding tension heads to *salvucci.xls*.

4. Compare the HYDRUS results with the tension heads calculated from Eq. (1), noting that Eq. (1) yields positive values and the values from HYDRUS are negative.

7.1.3 Expected Results

The HYDRUS simulations should agree with calculations using Eq. (1) within ± 10 percent for relatively low tension heads. Based on the findings of Salvucci (1993), the range of agreement should be better for the sandy loam soil than for the clay loam soil.

7.2 Test Case 2: Transient Flow Around a Land Mine

Test Case 2 compares a HYDRUS simulation with transient flow around a buried mine with results reported by Rhebergen, et al. (2002). This case was chosen to exercise the transient flow capability of HYDRUS and to test the radially symmetric mesh option. The model domain is illustrated in Figure 2. The domain has radial symmetry with a radius of 2 m [6.6 ft] and a depth of 2 m [6.6 ft]. A land mine, represented as a zone of very low saturated hydraulic conductivity {10^{-10} cm/s [4×10^{-11} in/s]}, is located at the center of the domain. The top of the land mine is at 30 cm [12 in] below the surface, and the bottom of the land mine is at 56 cm [22 in] below the surface. The rest of the model domain consists of homogeneous sand. The lower model boundary and right and left boundaries are defined as no flow. The upper model boundary is

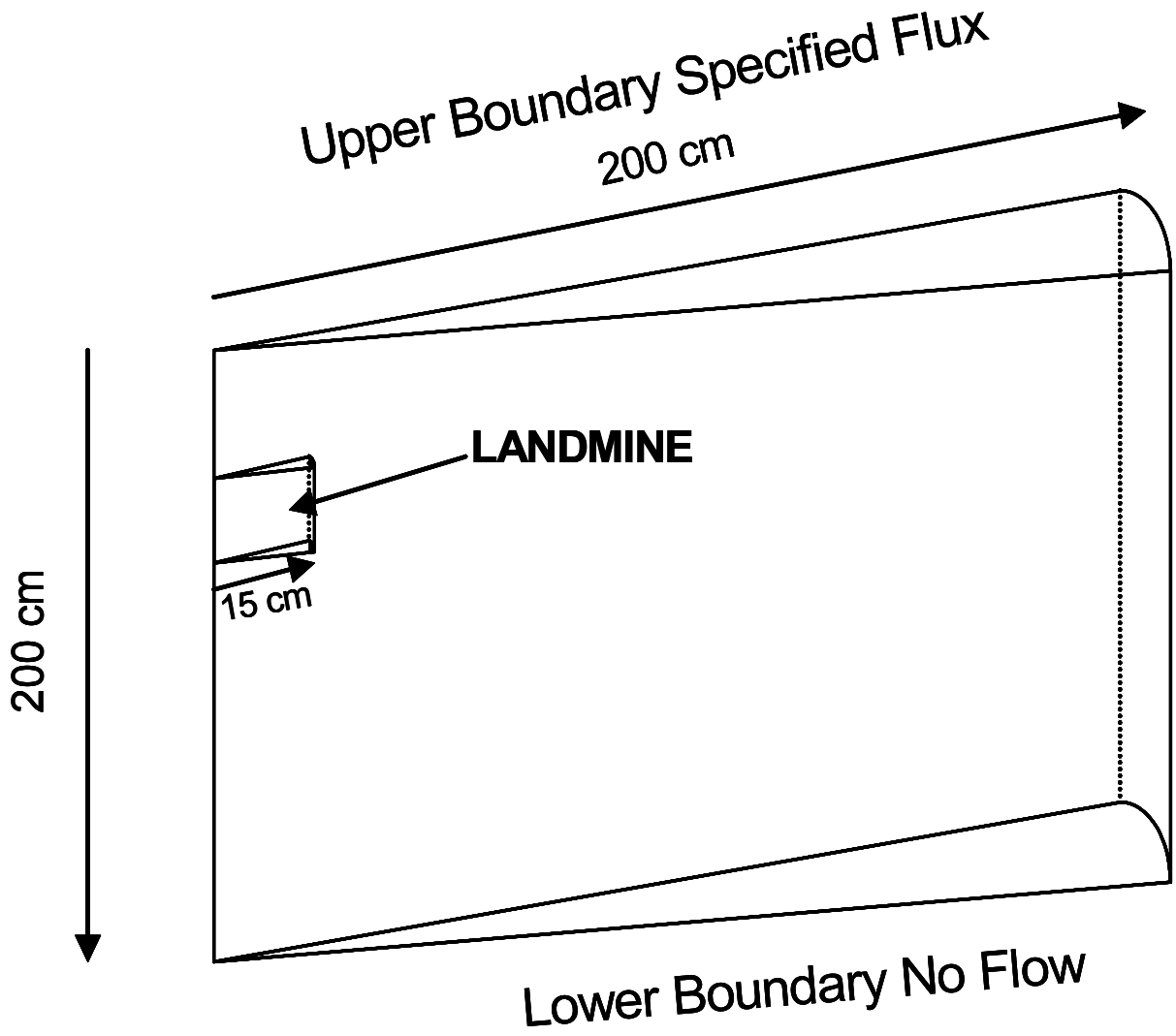

Figure 2. Model Domain and Boundary Conditions for Test 2 [1 cm = 0.39 in]

assigned a time-variable flux. The sand hydraulic properties are represented using the van Genuchten model given by

$$K(\psi) = K_s S_e^{\ell}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{5}$$

where

S_e	—	effective saturation
ℓ and m	—	empirical fitting parameters

The effective saturation in Eq. (5) is given by

$$S_e(\psi) = \left(1 + \left|\alpha\psi\right|^n\right)^{-m} \tag{6}$$

where

m	—	$1-1/n$
α	—	empirical fitting parameters

The hydraulic properties assigned to the sand are listed in Table 2.

The model domain is assigned an initial water content of 0.045. The simulation is started with the upper boundary flux set to zero. After 1 hour, the boundary flux is specified as 8 cm/hr [3.1 in/hr] for 1 hour. The boundary flux is set to zero starting at hour three of the simulation and held there for the rest of the simulation (4 days).

Observation nodes are assigned at depths of 10, 28, and 46 cm [3.9, 11, and 18 in] below the top of the model along the inner (x = 0) model boundary.

7.2.1 Input Files for Test Case 2

The HYDRUS input files for the land mine simulation are contained in directory *H3D_landmine*.

7.2.2 Test Procedure

1. Run the HYDRUS simulations.

2. Export the time histories of observation node water contents to *landmine_Observation_Nodels_Water_Content.xls*.

3. Compare the HYDRUS results with the results reported by Rhebergen, et al. (2002).

7.2.3 Expected Results

The HYDRUS results should be qualitatively reasonable and similar to those reported by Rhebergen, et al. (2002). The results may not exactly agree with Rhebergen, et al. (2002)

Table 2. Hydraulic Parameters Used for Test 2 Sand					
Residual Water Content	**Saturated Water Content**	**K_s (cm/s)***	**α (1/cm)***	**van Genuchten *n***	***l***
0.045	0.43	8.25×10^{-3}	0.145	2.68	0.5
*1 cm = 0.39 in					

because of uncertainties in the model construction and hydraulic properties used by Rhebergen, et al. (2002).

7.3 Test 3: One-Dimensional Transport Through a Semi-Infinite Column

Test 3 simulates one-dimensional mass transport through a soil column under steady flow conditions. The HYDRUS simulation results are compared to an analytical solution for transport of a tracer through a semi-infinite column including first-order decay (Javandel, et al., 1984) given by:

$$\frac{C(x,t)}{C_0} = \frac{v}{v+\beta}\exp\left\{\frac{x(v-\beta)}{2\delta v}\right\}erfc\left[\frac{xv-\beta t}{2(\delta vt)^{1/2}}\right] + \frac{v}{v-\beta}\exp\left\{\frac{x(v+\beta)}{2\delta v}\right\}erfc\left[\frac{xv+\beta t}{2(\delta vt)^{1/2}}\right] + \frac{v^2}{2\delta\lambda}\exp\left\{\frac{x}{\delta}-\lambda t\right\}erfc\left[\frac{xv+\beta t}{2(\delta vt)^{1/2}}\right] \quad (7)$$

where

$C(x,t)$	—	concentration at distance *x* from the upstream boundary and time *t*
C_0	—	upstream concentration
v	—	fluid pore velocity [cm/s]
δ	—	hydrodynamic dispersivity [cm]
λ	—	decay rate [1/s]

and

$$\beta = (v^2 + 4\delta v\lambda)^{1/2} \quad (8)$$

The analytic model is implemented in the spreadsheet *javandel.xls*.

The HYDRUS simulations are performed for a vertical soil column 1,000 cm [394 in] long and 10 cm [3.9 in] wide. The vertical node spacing is 10 cm [3.9 in]. A constant water flux is assigned into the upper boundary and a corresponding flux out of the lower boundary. A constant concentration of tracer is introduced into the upper boundary after steady water flow conditions are established in the column. The soil column is assigned the default hydraulic

properties of a loamy sand listed in Table 3, and the van Genuchten hydraulic model is used to compute unsaturated hydraulic properties. The concentration distribution computed by HYDRUS is output at selected times before the concentration front contacts the lower boundary to approximate a semi-infinite flow domain. HYDRUS provides three options for solving the transport problem: (i) Galerkin finite element formulation, (ii) upstream weighting of the finite element formation, and (iii) Galerkin method with artificial dispersion. The latter two options are used to reduce numerical oscillations at large Peclet numbers. Simulations are run using each of these options and compared to the analytical solution with the decay rate set to zero. One simulation is run with a nonzero decay rate using the Galerkin formulation. The simulations are run using a dispersivity of 1 cm [0.39 in] resulting in a grid Peclet number of 10.

7.3.1 Input Files for Test Case 3

The HYDRUS input files for the land mine simulation are contained in directory *H3D_1-dtransport*.

7.3.2 Test Procedure

1. Run HYDRUS to simulate 10 days using constant water flux of 1.0×10^{-3} cm/s [3.9×10^{-4} in/s] at influent and effluent boundaries to establish steady flow conditions.

2. Assign the water content generated by Step 1 as the initial condition to the transport simulation.

3. Run the HYDRUS simulations with an input concentration of 1.0 using each of the solution methods and with the decay constant set to zero. Run a simulation using the Galerkin formulation and a decay constant of 1×10^{-5} 1/second.

4. Export the vertical concentration distributions at times when the tracer pulse has moved approximately halfway through the column using the “cross-section” extraction tool in HYDRUS.

5. Copy the concentration distribution to the spreadsheet *javandel.xls*.

6. Compare the HYDRUS results with the results computed by the Javandel solution.

Table 3. Hydraulic Parameters Used for Test 3 Loamy Sand

Residual Water Content	Saturated Water Content	K_s (cm/s)*	α (1/cm) *	van Genuchten *n*	*l*
0.057	0.41	4.05×10^{-3}	0.124	2.28	0.5

*1 cm = 0.39 in

7.3.3 Expected Results

For the case of no decay, the position of the HYDRUS 0.5 concentration value should be within ±10 percent of that computed using the analytic solution. The Galerkin method may display oscillations at high and low concentrations. The other methods may display numerical dispersion relative to the analytic solution. The simulated concentrations with decay should agree with the analytic solution within ±10 percent.

8 RESULTS

The methods and results of the validation are contained in Scientific Notebook 813.

8.1 Test Case 1: Steady-State Tension Head Distribution in Vertical Column

The simulations for Test Case 1 were performed on August 2, 2006. The resulting input and output files are in directories *H3D_1-dsalvucci clay loam*, *H3D_1dsalvucci sand loam*, and *salvucci* on the HYDRUS validation CD in Scientific Notebook 813. The comparisons between the tension heads computed by HYDRUS and those computed using the Salvucci analytical models are shown in Figures 3 and 4 for the sandy loam and clay loam models, respectively. The HYDRUS results agree with the Salvucci analytical solution for the sandy loam within ±10 percent. For clay loam, the HYDRUS results agree with the Salvucci solution within ±10 percent for low values of tension head, but diverge somewhat for larger tension heads. This behavior is consistent with the approximations in the Salvucci solution and is consistent with the results reported by Salvucci (1993). The validation test is considered to be acceptable.

8.2 Test Case 2: Transient Flow Around a Land Mine

The simulations for Test Case 2 were run on August 3, 2006, and are described in Scientific Notebook 813. The input and output files for this test case are contained in directories *H3D_landmine*, and *landmine* on the HYDRUS validation CD in Scientific Notebook 813. Simulated time histories of water content at locations approximately corresponding to those reported by Rhebergen, et al. (2002) are shown in Figure 5. The spatial distribution of water content after 21,600 seconds (6 hours) is shown in Figure 6. The HYDRUS results are consistent with, but slightly different than, those reported by Rhebergen, et al. (2002). For the 10-cm [3.9-in]-depth observation point, the peak in the water content occurs almost immediately after the onset of water application (Figure 5) and has a value of 0.35, consistent with the results of Rhebergen, et al. (2002). After 48 hours, however, the water content at the 10 cm [3.9 in] observation point approaches 0.09 as opposed to 0.15 as reported by Rhebergen, et al. (2002). The peak of the 28-cm [11-in] water content occurs slightly later than the 10-cm [3.9-in] peak, which is consistent with the results of Rhebergen et al. (2002) for 30 cm [12 in]. The 28-cm [11-in] peak is 0.43 compared to 0.35 reported by Rhebergen, et al. (2002). The 46-cm [18-in] water content does not begin to increase until 6 hours into the simulation whereas Rhebergen, et al. (2002) reported that the water content did not begin to increase until 11 hours at the 45-cm [18-in] depth. Given that the finite element grid used in the simulation was not identical to that of Rhebergen, et al. (2002) and there is some ambiguity in the soil hydraulic properties used by Rhebergen, et al. (2002), the validation results are reasonable. The water content distribution shown in Figure 6 is also conceptually reasonable, showing the shadowing

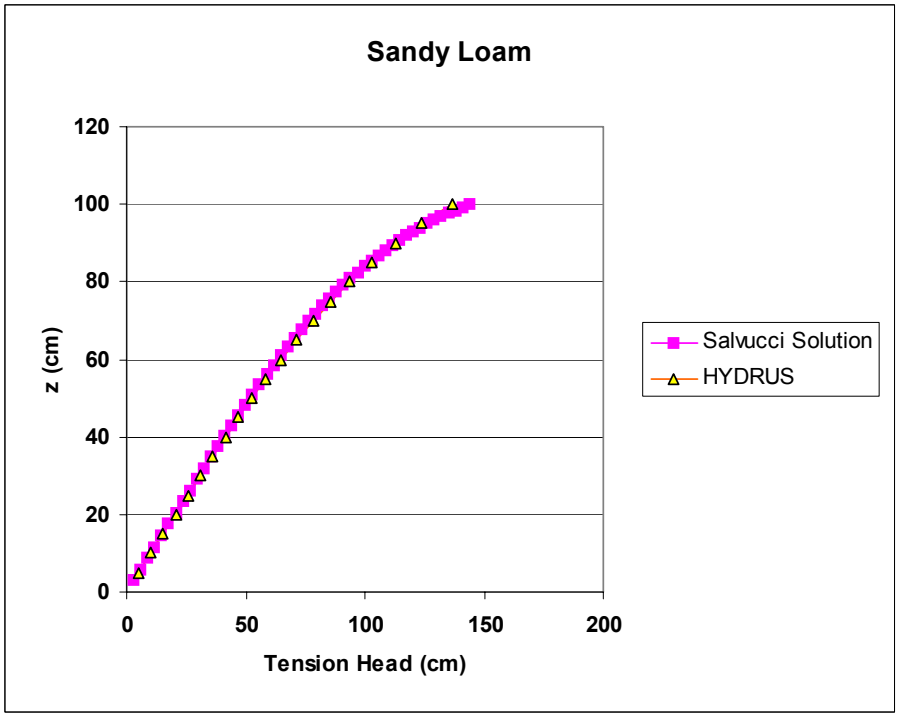

Figure 3. Comparison of Tension Head Computed Using HYDRUS With Tension Head Computed Using Salvucci Analytical Solution for Sandy Loam [1 cm = 0.39 in]

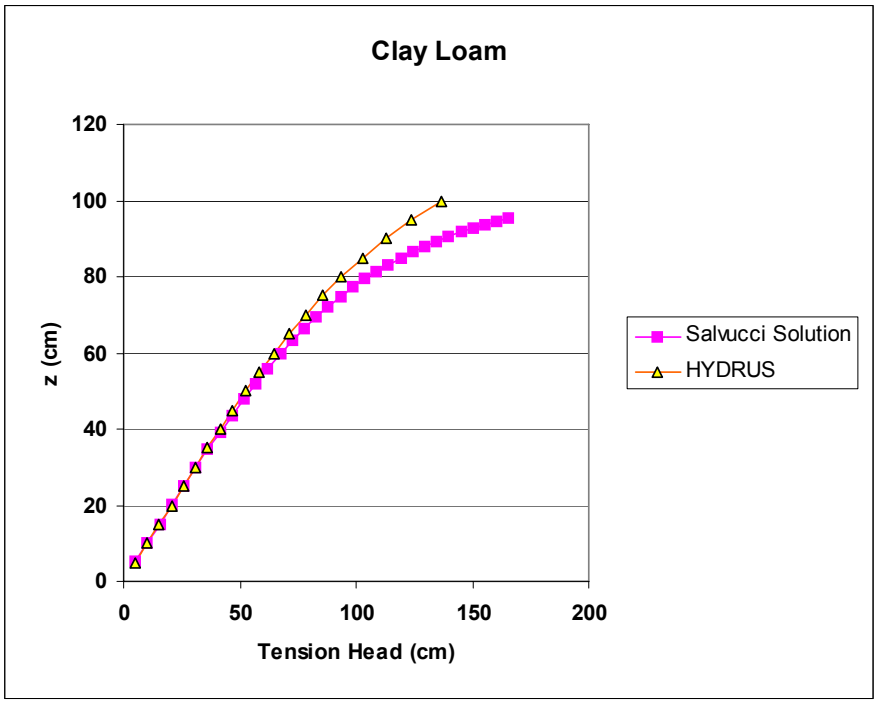

Figure 4. Comparison of Tension Head Computed Using HYDRUS With Tension Head Computed Using Salvucci Analytical Solution for Clay Loam ([1 cm = 0.39 in]

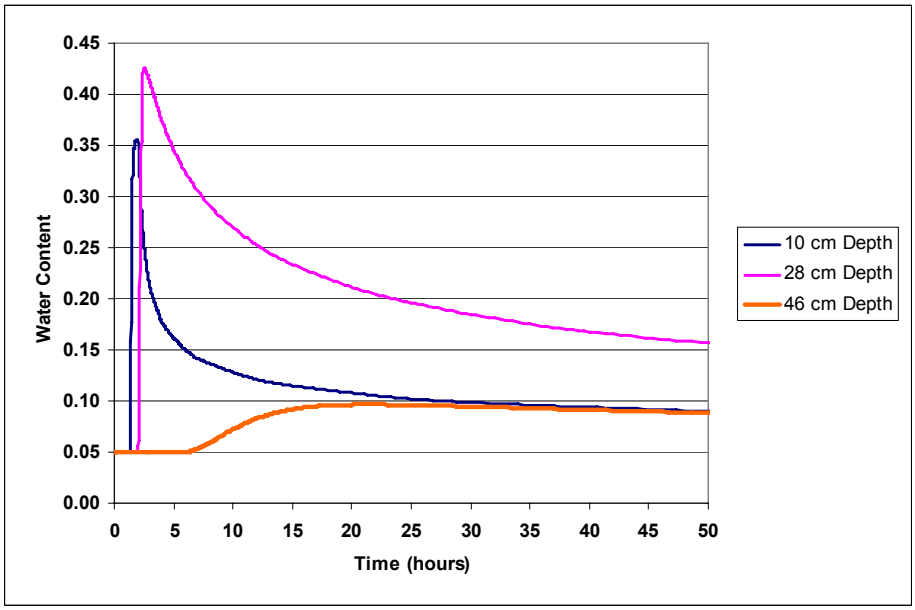

Figure 5. Simulated Change in Water Content at Selected Depths Computed by HYDRUS [1 cm = 0.39 in]

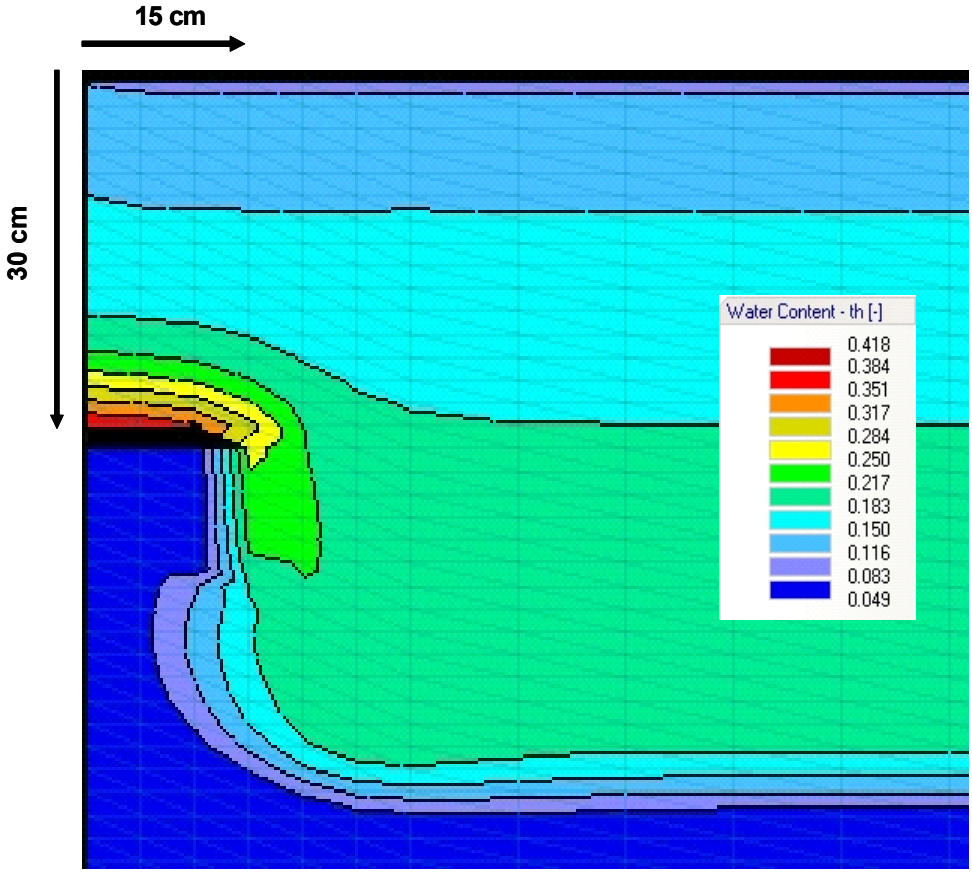

Figure 6. Simulated Distribution of Water Content After 21,600 Seconds Computed by HYDRUS [1 cm = 0.39 in]

effect of the land mine. Based on these considerations, the results of the validation test are acceptable.

8.3 Test Case 3: One-Dimensional Transport Through a Semi-Infinite Column

The simulations for Test Case 3 were run on August 14, 2006, and are described in Scientific Notebook 813. The input and output files for this test case are contained in directories *H3D_1-dtransport* and *analytic* on the HYDRUS validation CD in Scientific Notebook 813. The results of the transport simulations without decay are shown in Figure 7 along with the analytical solution programmed in *javandel.xls* for the simulation time of 178,200 seconds. The results for the upstream weighted finite element formation and the Galerkin method with artificial dispersion were practically identical, and only results for the upstream weighted finite element formulation are shown. Overall, the HYDRUS results agree reasonably well with the analytic solution and differ in a manner to be expected based on the numerical solution methods. The Galerkin method agrees quite well with the analytical solution between relative concentrations of 0.9 and 0.1, but shows an oscillation at relative concentrations greater than 0.9. This is to be expected for the relatively large grid Peclet number (10) used in the model. The upstream weighted method displays numerical dispersion but no oscillation, which is also to be expected.

The results for the simulation using the Galerkin method and a decay constant of 1×10^{-5} 1/s are shown in Figures 8 and 9. The HYDRUS results agree with the analytical solution within ±10 percent down to a relative concentration of 1×10^{-2}. Below that relative concentration, the HYDRUS results are probably affected by some numerical dispersion.

Overall, the HYDRUS results agree well with the analytical solution with the limits of the numerical methods, and the validation results are acceptable.

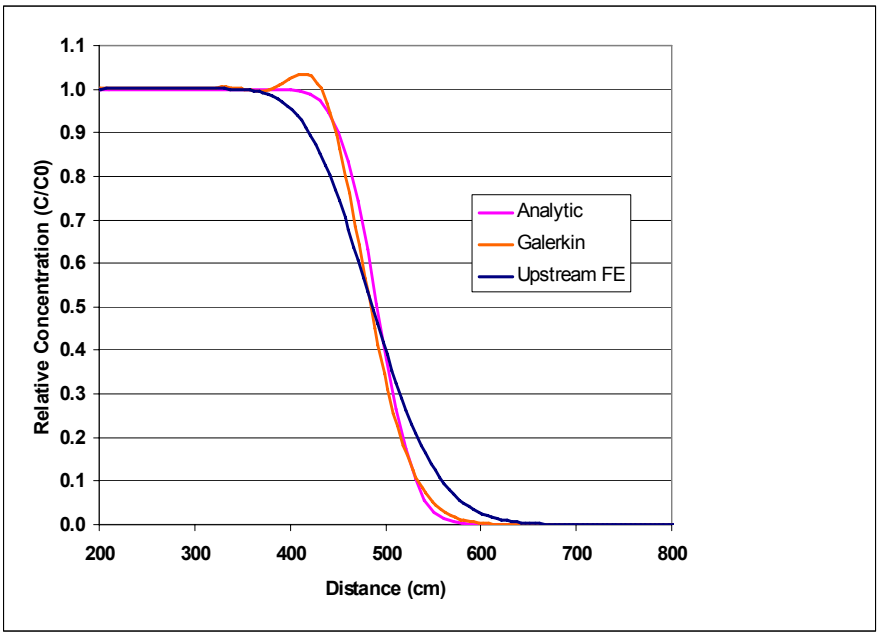

Figure 7. Comparison of HYDRUS Simulation Results Using Galerkin and Upstream Weighted Finite Element Methods With Analytic Solution at Simulation Time Equal to 178,200 Seconds [1 cm = 0.39 in]

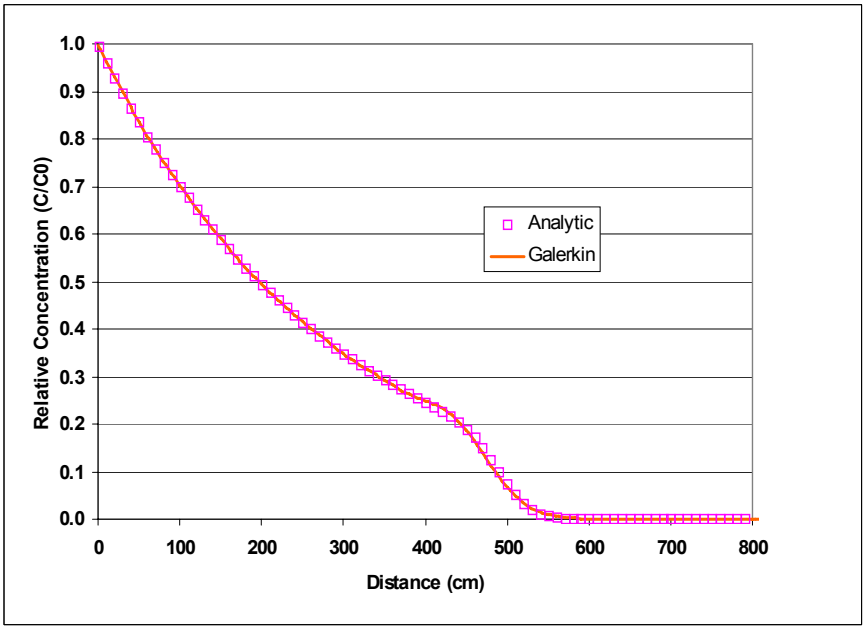

Figure 8. Comparison of HYDRUS Simulation Results Using Galerkin Method for Decay Constant Equal to 1×10^{-5} 1/second With Analytic Solution at Simulation Time Equal to 178,200 Seconds (Arithmetic Scales) [1 cm = 0.39 in]

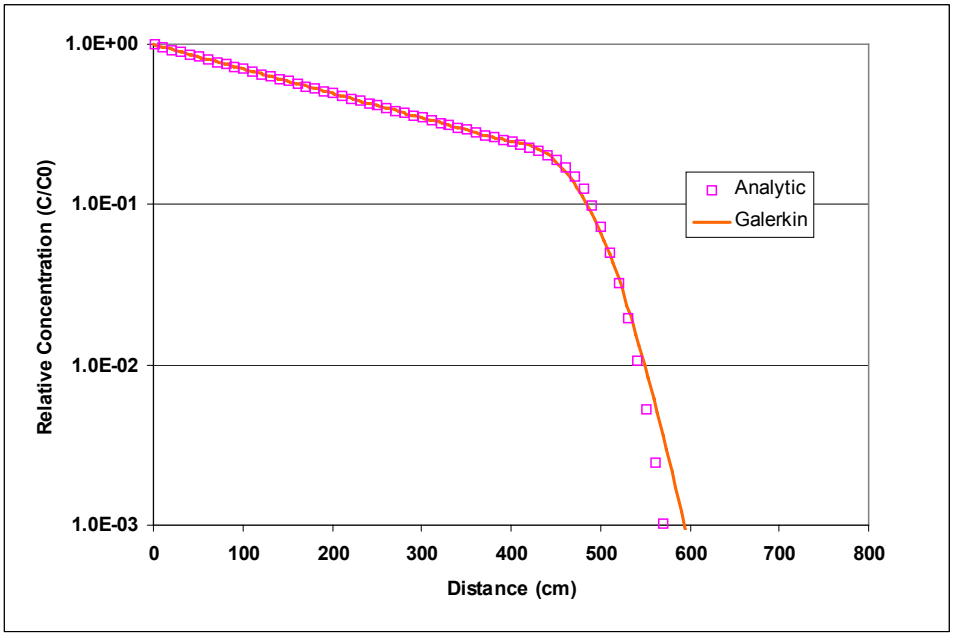

Figure 9. Comparison of HYDRUS Simulation Results Using Galerkin Method for Decay Constant Equal to 1×10^{-5} 1/seconds With Analytic Solution at Simulation Time Equal to 178,200 Seconds (Log Scale) [1 cm = 0.39 in]