SOFTWARE VALIDATION TEST PLAN AND REPORT FOR GEOSTUDIO™ VADOSE/W© 2007 VERSION 7.11

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This is a software validation test plan and report for acquired software GeoStudio™ VADOSE/W© 2007 Version 7.11 (GEO-SLOPE International, Ltd., 2007). Henceforth, this software will be referred to as VADOSE/W. VADOSE/W is a two-dimensional, simultaneous coupled heat transport and fluid flow finite element model for vadose zone hydrological processes that rigorously couples soil hydraulic behavior with atmospheric forcing or climate conditions. Major physical processes that VADOSE/W can model include actual evaporation, plant transpiration, plant growth, surface runoff, ponding, lateral flow redistribution, infiltration, water percolation, vapor flow, gas diffusion, heat transfer, aqueous phase change, snow accumulation, ablation, and melt.

This report conforms to the software validation requirements of Technical Operating Procedure (TOP)–018—Development and Control of Scientific and Engineering Software. Software is validated to gain confidence that software successfully implements its underlying theory and algorithms. Software validation test plans describe test cases that will provide evidence supporting the correct and successful implementation of the software functions, often including comparative test cases (analytical or numerical) that can be used to benchmark software performance. When available and applicable, the software validation test plan may describe benchmark data or solutions from published research papers, published laboratory experimental results, or existing test cases.

The three initial selected test cases (Test Cases 1–3) were designed to determine whether the main software functions are properly and correctly implemented. One test case (Test Case 3) revealed that VADOSE/W is not currently designed to model cryosuction and resultant moisture flow toward a freezing front. Due to this singular negative result, three additional test cases (Test Cases 4–6) involving freezing or thawing were added to the original set of validation test cases to confirm that simple phase change processes are appropriately handled. The resulting software validation suite of test cases (Table 1) compares VADOSE/W solutions with published solutions, with the exception of one hypothetical soil cover test case (Test Case 2) focused on demonstrating that the software appropriately conserves mass. Different degrees of expected agreement between VADOSE/W simulations and published solutions are based on a qualitative assessment of the accuracy of independent models, considering the approximations they include, and the reasonable accuracy expected from VADOSE/W given the assumptions on which its algorithms are based.

This report is organized consistent with the existing template for all such software validation exercises. Section 1 provides the scope of the validation; Section 2 lists the report references; Section 3 describes the software and hardware environment associated with validation testing; Section 4 describes software assumptions and any constraints, and Section 5 describes the test cases used to validate the functionalities of the software and the results of the validation tests. Per request by U.S. Nuclear Regulatory Commission (NRC) staff, conclusions are provided in Section 6, and an appendix provides additional supporting information for the approach taken for the VADOSE/W software validation.

Table 1. Physical Processes Enabled for Each Test Case										
Test Case	**Evaporation**	**Transpiration**	**Plant Growth**	**Surface Runoff**	**Lateral Water Redistribution**	**Infiltration**	**Percolation**	**Gas Diffusion**	**Phase Change**	**Heat Transfer**
1	X									
2	X	X	X	X	X	X	X	X	X	X
3									X	X
4									X	X
5									X	X
6									X	X

1 SCOPE OF VALIDATION

VADOSE/W was primarily developed to assist in the design of engineered soil cover systems. VADOSE/W is accompanied by a variety of illustrative examples that can be used to validate the software (GEO-SLOPE International, Ltd., 2007, Chapter 11). VADOSE/W includes a wide range of features, not all of which are addressed directly via this validation exercise. The scope of this validation is limited to (i) a one-dimensional evaporation test; (ii) a volumetric water balance review of a fully coupled, two-dimensional engineered soil cover model with transient climate boundary condition; (iii) a freezing soil vertical column test; (iv) a freezing column test with no water redistribution; (v) a thawing column test with no water redistribution; and (vi) a two-dimensional pipeline freezing analysis. These validation tests are considered appropriate for validating the capability of the code to simulate the relevant processes near engineered soil covers of most sites.

Specific validation simulations include

- Test Case 1: Simulation of steady-state pressure head distribution in a soil column with steady evaporation (Salvucci, 1993)
- Test Case 2: Simulation and volumetric water balance review of a transient, fully coupled, two-dimensional engineered soil cover with transient climate boundary condition
- Test Case 3: Simulation of a laboratory freezing soil experiment with convective heat transfer boundary condition and water redistribution (Hansson, et al., 2004)
- Test Case 4: Simulation of phase change under freezing conditions (Nixon and McRoberts, 1973)
- Test Case 5: Simulation of phase change under thawing conditions (Hwang, et al., 1972)
- Test Case 6: Simulation of frost bulb development around a buried pipeline (Coutts and Konrad, 1994)

The features and options of VADOSE/W not specifically considered in this validation should be tested as specific modeling needs arise.

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3 ENVIRONMENT

3.1 Software

GeoStudio VADOSE/W 2007 Version 7.11 (Build 4199) was obtained from GEO-SLOPE International, Ltd., Calgary, Alberta, Canada. The program was installed on a personal computer with Microsoft® Windows® XP Professional Version 2002 operating system. Postprocessing of output was performed with either VADOSE/W or with Microsoft Excel® 2002 SP3.

3.2 Hardware

VADOSE/W validation simulations were performed on the personal computer “Atlantis” with a 2.80 GHz Intel® Pentium® IV central processing unit.

4 ASSUMPTIONS AND CONSTRAINTS

VADOSE/W is a two-dimensional, simultaneous coupled heat transport and fluid flow finite element model for vadose zone processes that rigorously couples soil hydraulic behavior with atmospheric forcing or climate conditions. The flow equation is based on the Richards’ (1931) equation, but is adapted to include vapor flow according to the method of Wilson (1990) with a modification according to the method of Milly (1982). The heat transfer equation is based on the standard Fourier equation for conductive heat transfer, with modifications for inclusion of vapor and convective heat transfer (due to flowing water).

5 TEST CASES

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

Test Case 1 compares VADOSE/W results with an approximate analytical solution by Salvucci (1993) for the vertical tension head distribution in a homogeneous soil column with constant evaporation at its upper surface. A soil column of silt and a soil column of silty clay are modeled separately. See Walter (2006) for a similar validation test case using HYDRUS Version Beta.03. Salvucci’s solution in terms of elevation and tension head is

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

where

z	—	vertical coordinate [m]
ψ_1	—	bubbling head [m]
q'	—	ratio of surface flux, q [m/s], to saturated hydraulic conductivity, K_S [m/s]
ψ	—	tension head at z [m]
n	—	empirical coefficient, which relates hydraulic conductivity to tension head [dimensionless]

Salvucci's solution (1993) assumes 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 this surface evaporation analytical solution, the surface flux, q, is taken as positive and the lower boundary of the soil column is saturated [i.e., $\psi(z = 0) = 0$ as at a water table]. The empirical coefficients n [see Eqs. (1) and (2)] are determined for a silt and a silty clay given the hydraulic conductivity functions assumed within VADOSE/W. The Salvucci n parameters are determined within the spreadsheet *Salvucci.xls* using the Microsoft Excel Solver to maximize the R^2 for the correlation between the VADOSE/W-calculated hydraulic conductivity function and the function described by Eq. (2). Salvucci's n parameters for the selected silt and silty clay were found to be 1.069 and 1.027. The Salvucci analytical solution for z in terms of ψ is also implemented in the spreadsheet *Salvucci.xls* and will be discussed later.

VADOSE/W simulations for this transient, one-dimensional test case use the 1-m-high by 0.1-m-wide [3.3-ft-high by 0.33-ft-wide] rectangular grid of finite element quadrilaterals shown in Figure 1. The nonsurface-layer mesh consists of 1 element in the horizontal direction and 39 elements in the vertical direction. The surface-layer mesh consists of 1 element in the horizontal direction and 2 elements in the vertical direction.

Simulations are performed for silt {bubbling head = 2.5 kPa [0.36 psi]} and silty clay {bubbling head = 1.4 kPa [0.20 psi]} using soil moisture curve sample functions provided in VADOSE/W. Saturated volumetric water contents (θ_S) for the silt and silty clay were assumed at 0.3 and 0.6. Minimum and maximum suctions for both the silt and silty clay are assumed at 0.01 and 100 kPa [14.5 psi]. Compressibility (*Mv*) is assumed at 1×10^{-5} kPa^{-1} [6.9×10^{-5} psi^{-1}] for all cases. The material properties of the surface layer do not differ from those of the non-surface layer for this test case. VADOSE/W estimates the hydraulic conductivity function from the soil moisture curve using the van Genuchten (1980) estimation method for this test case. Saturated hydraulic conductivities (K_S) for the silt and silty clay are assumed at 7.19×10^{-6} and 6.39×10^{-7} m/s [2.36×10^{-5} and 2.10×10^{-6} ft/s]. The residual water content is estimated at 0.0167 for both soils.

The lower boundary condition is a constant tension head of 0 m [0 ft]. The upper boundary condition is a constant evaporative flux of -1.58×10^{-8} m/s [5.18×10^{-8} ft/s], which is equivalent to −0.5 m/yr [−1.6 ft/yr].

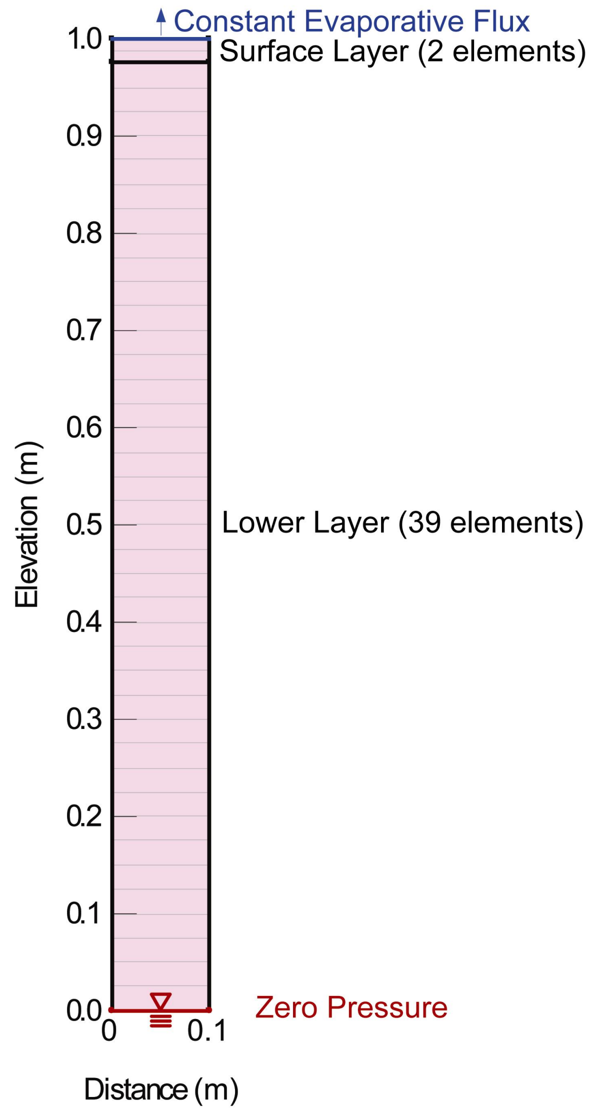

Figure 1. Rectangular Grid of Finite Element Quadrilaterals VADOSE/W Used in the Implementation of Test Case 1

For two simulations, an initial water table will be specified (a common approach employed within VADOSE/W) at the lower boundary, which when combined with the soil moisture curve, yields a physically based initial pore water pressure condition. For two additional simulations, in lieu of setting an initial water table initial condition, the material activation pore water pressure will be set to −9.81 kPa [−1.42 psi] for both layers, which is equivalent to setting the tension head throughout the model domain to an initial condition of −1 m [−3.3 ft], as Walter (2006) did when validating HYDRUS with a similar test case.

5.1.1 Test Procedure

1. In VADOSE/W: Set units and scale; draw model geometry; specify material properties (including initial condition) and boundary conditions; mesh model domain; establish adaptive timestepping.

2. Run VADOSE/W simulations for 8.64×10^5 seconds (10 days) to establish quasi-steady-state conditions.

3. Export final tension heads as a function of elevation from VADOSE/W simulations to a Microsoft Excel spreadsheet file named *Salvucci.xls*: spreadsheet tab labeled either "Silty Clay Comparison" or "Silt Comparison," as appropriate.

4. Determine the Salvucci *n* parameters within the spreadsheet *Salvucci.xls* using the Microsoft Excel Solver to maximize the R^2 for the correlation between the VADOSE/W-calculated hydraulic conductivity function and the function Eq. (2) described.

5. Solve for *z* in terms of ψ using the Salvucci analytical solution [Eq. (1)] in the spreadsheet *Salvucci.xls*: spreadsheet tabs labeled either "Silty Clay Comparison" or "Silt Comparison."

6. Compare VADOSE/W results with the tension heads calculated from Eq. (1), noting that Eq. (1) yields positive tension head values, whereas VADOSE/W tension head values are negative in sign.

5.1.2 Results

The VADOSE/W simulations should agree with calculations using Eq. (1) within ±10 percent for relatively low tension heads. Based on the findings of Salvucci (1993), agreement should be better for the silt than for the silty clay.

The simulations for Test Case 1 were performed on June 2, 2008. Analytical and numerical results are contained in Microsoft Excel file *Salvucci.xls* and VADOSE/W file *Validation Exercise Salvucci 1993.gsz* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008). Four separate analyses are contained within the VADOSE/W file: (i) *VADOSE/W Salvucci Analysis 1993 (Silt)* (uses initial water table as initial condition instead of material activation pore water pressure); (ii) *VADOSE/W Salvucci Analysis 1993 (Silt) (2)* {uses constant −9.81 kPa [−1.42 psi] or −1 m [−3.3 ft] material activation pore water pressure as initial condition instead of initial water table}; (iii) *VADOSE/W Salvucci Analysis 1993 (Silty Clay)* (uses initial water table as initial condition instead of material activation pore water pressure); and (iv) *VADOSE/W Salvucci Analysis 1993 (Silty Clay) (2)* {uses constant −9.81 kPa [−1.42 psi] or −1 m [−3.3 ft] material activation pore water pressure as initial condition instead of initial water table}. While the final results were the same regardless of specified initial condition, the number of timesteps required to reach steady state were much reduced when specifying an initial water table.

VADOSE/W simulations for a given soil type using either initial condition converged to the same solution for tension head as a function of elevation and material. The comparisons between the tension heads VADOSE/W computed and those computed using the Salvucci analytical solution are shown in Figure 2 for the silt and silty clay models. The VADOSE/W silt results agree with the Salvucci analytical solution within 1.2 percent, and the silty clay results agree within 6.6 percent, where percent error is calculated as $100 \times$ [(estimated value − true value)/true value)] and the estimate comes from VADOSE/W, whereas the true value comes from a published solution. The results of this validation test are acceptable.

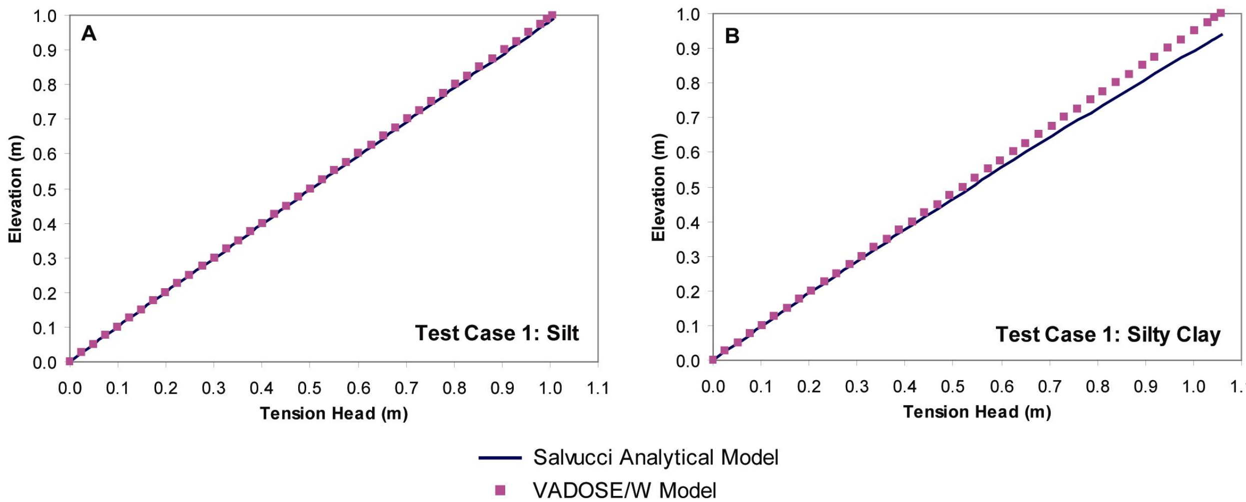

Figure 2. Test Case 1: Comparison of Tension Head VADOSE/W Computed With Tension Head Computed Using Salvucci (1993) Analytical Solution for (A) a Silt and (B) a Silty Clay [1 m = 3.3 ft]

5.2 Test Case 2: Simulation and Volumetric Water Balance Review of a Transient, Fully Coupled, Two-Dimensional Engineered Soil Cover With Transient Climate Boundary Condition

Test Case 2 creates a transient, fully coupled, two-dimensional engineered soil cover model with a Spokane, Washington, climate boundary condition applied on a variably sloped topographic surface. These climate data are available via GEO-SLOPE International, Ltd. The Test Case 2 numerical model checks several VADOSE/W capabilities, and the validation will be realized through analysis of the volumetric water balance results. Vegetation is included with the climate boundary condition; oxygen diffusion is modeled; and soil freezing processes are allowed but do not dominate, because the selected climate data do not support freezing.

VADOSE/W simulations for this test case use the geometry and mesh shown in Figure 3. The nonsurface layer is gridded with an unstructured quadrilateral and triangle element mesh. The surface layers are gridded with a quadrilateral element mesh with vertically oriented nodes.

Material properties are defined for the (i) waste material, (ii) compacted low hydraulic conductivity engineered cover, (iii) near-subsurface growth layer, and (iv) surface growth layer. The soil moisture curves for both growth layers are identical, but the hydraulic conductivity function for the surface layer is constrained to vary by only three orders of magnitude, which allows for larger hydraulic conductivities at the surface due to desiccation cracks and other such large-scale surface void features. The soil moisture curves and hydraulic conductivity functions assigned to the various material layers are shown in Figure 4. VADOSE/W estimates the nonsurficial hydraulic conductivity functions from the defined soil moisture curves using the van Genuchten (1980) estimation method with user-defined modifications for this test case. The surficial conductivity function is constrained within VADOSE/W by repicking conductivity data points at large suctions such that they vary by no more than three orders of magnitude.

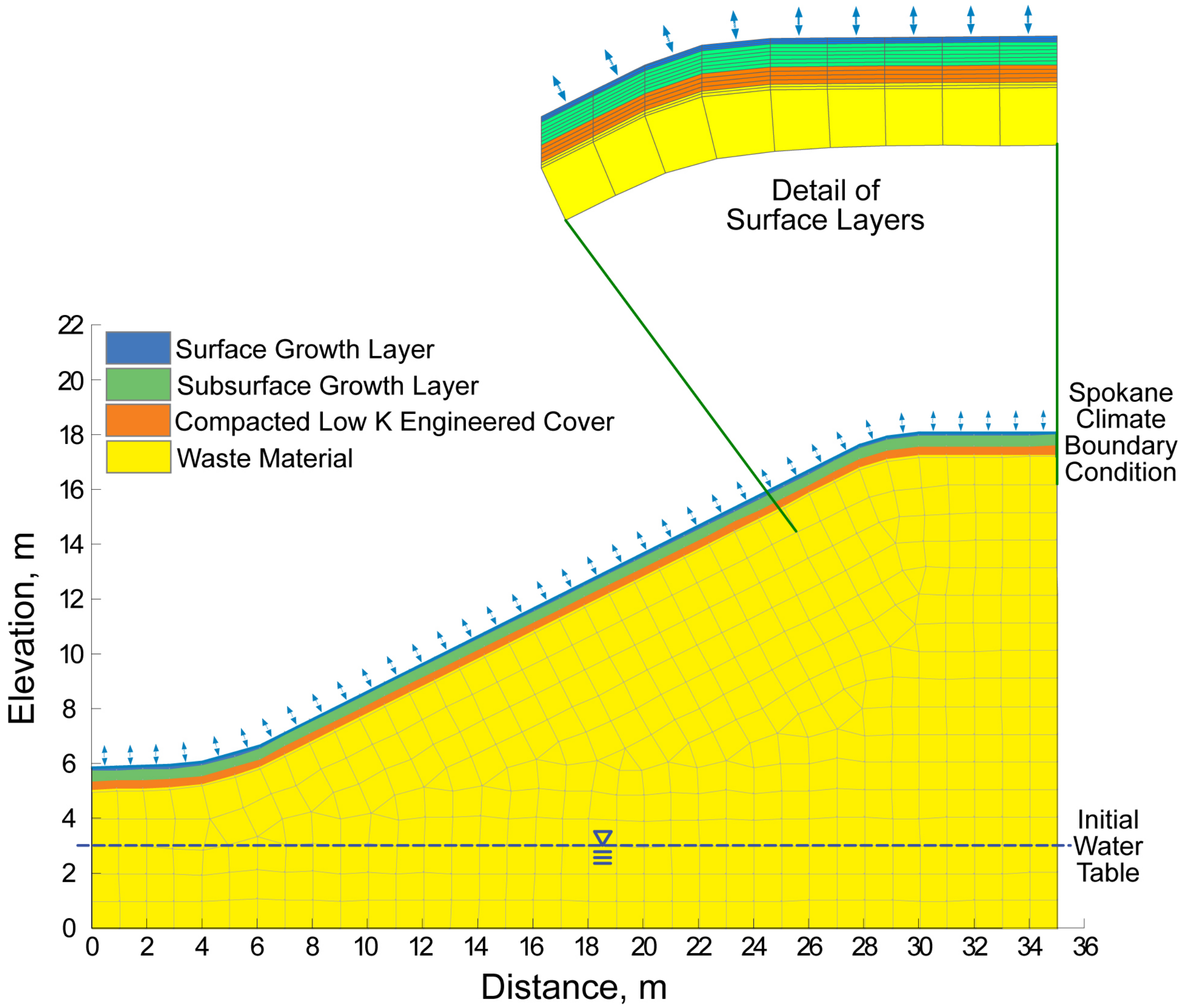

Figure 3. Model Geometry and Unstructured Quadrilateral and Triangle Element Mesh VADOSE/W Used in the Implementation of Test Case 2

The climate boundary condition consists of meteorological data from Spokane, Washington. The complete climate data set spans the dates May 1, 1994, to May 1, 1995, but the numerical model is initiated on Day 100 and ends on Day 130. The entire climate data set is contained within the VADOSE/W *Test Case 2.gsz* file on the CD associated with Scientific Notebook 933E (Dinwiddie, 2008). Because vegetation is included in the model, three vegetation functions are defined: (i) the leaf area index, (ii) the moisture-limiting factor function, and (iii) the root depth over growing season function. The functions defined for use in the model are shown in Figure 5.

The initial hydrologic condition for this simulation is defined by an initial water table located 3 m [10 ft] above the base of the model domain, as shown previously in Figure 3. The material activation temperature initially assigned to all material layers is 10 °C [50 °F]. The material activation oxygen gas concentration initially assigned to each layer is 0 g/m^3 [0 lb_m/ft^3].

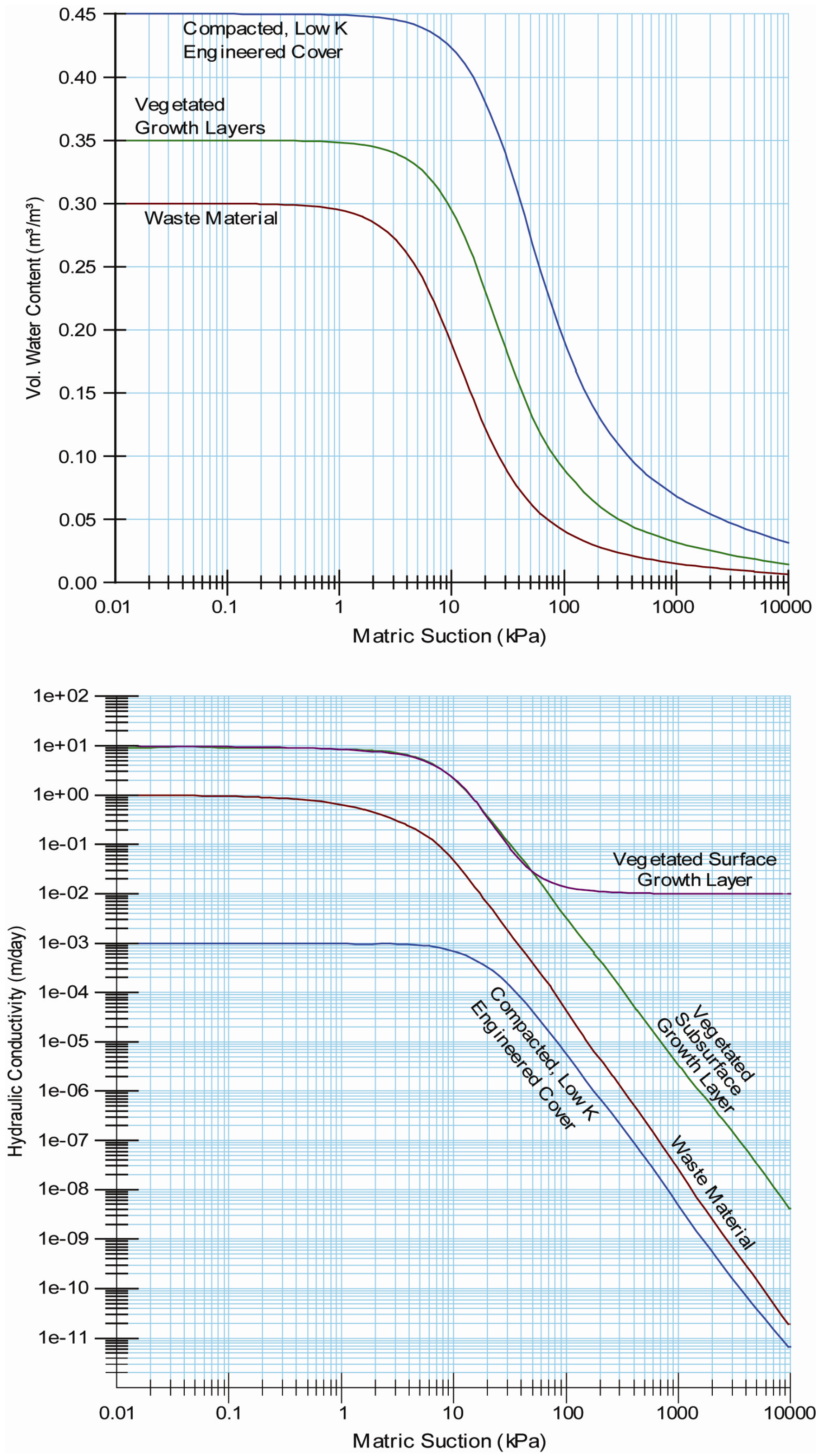

Figure 4. Soil Moisture Curves and Hydraulic Conductivity Functions Assigned to Model Layers in the Implementation of Test Case 2

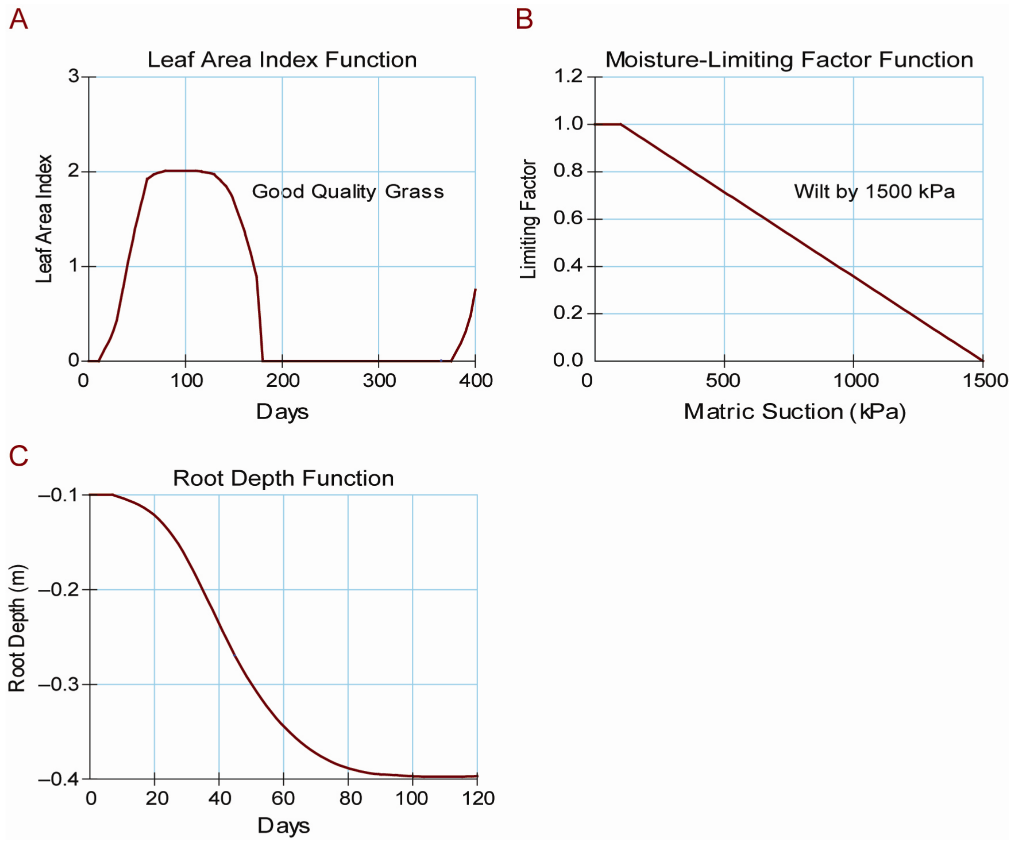

Figure 5. Vegetation Functions Assigned to the Climate Boundary Condition in the Implementation of Test Case 2: (A) Leaf Area Index Function for Good Quality Grass, (B) Moisture-Limiting Factor Function Defines 1,500 kPa [218 psi] as the Wilting Point, and (C) Root Depth Over Growing Season Function

5.2.1 Test Procedure

1. In VADOSE/W: Set units and scale; establish 30 timesteps (daily), establish adaptive timestepping, and require results to be saved every second day; draw model geometry including four distinct soil layers (waste material, compacted clay layer, subsurface growth layer, and surface growth layer); specify material properties, boundary conditions (using Spokane, Washington, climate data and constructed vegetation functions), and initial conditions; mesh model domain.

2. Run VADOSE/W simulation for Climate Days 100 to 130.

3. Analyze resulting volumetric water balance using convergence data and graphing capabilities within VADOSE/W. Export water balance graphics to reports and compare water balance error to volume of total precipitation input to model domain over modeling period.

5.2.2 Results

The VADOSE/W simulation should result in the recording of convergence data at the end of each of 30 converged timesteps. The convergence data are cumulative and apply to the entire model domain. The volumetric water balance graphic will include categories for precipitation, actual evaporation, actual transpiration, other boundary fluxes, and changes in storage. The sum of these quantities should be zero, or if finite, this sum constitutes the water balance error in the numerical model (i.e., change in storage + precipitation + boundary flux in – actual evaporation – plant transpiration – runoff – boundary flux out = water balance error). This validation exercise will be found satisfactory if the cumulative volumetric water balance error for the model domain is less than 2 percent of the cumulative precipitation over the model domain.

The simulations for Test Case 2 were performed on June 5, 2008. Numerical results are contained in VADOSE/W file *Test Case 2.gsz* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008). The volumetric water balance results are displayed in Figure 6. The cumulative water balance error has an absolute value of 0.00013 m^3 [0.00459 ft^3], which is only 0.02 percent of the total precipitation {0.58 m^3 [21 ft^3]} input to the model domain over the simulation period. The results of this validation test are acceptable.

5.3 Test Case 3: Simulation of a Laboratory Freezing Soil Experiment With Convective Heat Transfer Boundary Condition and Water Redistribution

Test Case 3 simulates a laboratory freezing soil experiment by Mizoguchi (1990) with convective heat transfer at its upper surface. The laboratory experiment specifications are detailed in Hansson, et al., (2004). The Test Case 3 numerical model checks the VADOSE/W water redistribution capability at a freezing front by comparing VADOSE/W results against experimental results documented in Hansson, et al. (2004).

VADOSE/W simulations for this transient, one-dimensional test case use the 0.2-m-high by 0.08-m-wide [0.7-ft-high by 0.3-ft-wide] rectangular grid of finite element quadrilaterals shown in Figure 7. The nonsurface-layer mesh consists of 1 element in the horizontal direction and 19 elements in the vertical direction. The surface-layer mesh consists of 1 element in the horizontal direction and 5 elements in the vertical direction.

Simulations are performed for Kanagawa sandy loam soil using soil moisture and unsaturated conductivity functions measured by Ishida (1983) and modeled with van Genuchten's (1980) analytical model (Hansson, et al., 2004, Figure 3). As reported in Hansson, et al. (2004), the model fit to the Ishida (1983) data resulted in the following parameters: $\theta_r = 0.05$, $\theta_s = 0.535$, $K_s = 3.2 \times 10^{-6}$ m·s^{-1} [1.0×10^{-5} ft·s^{-1}], $\alpha = 1.11$ m^{-1} [0.34 ft^{-1}], $n = 1.48$, and $m = 0.2$. Note that Hansson, et al. (2004) did not set $m = 1 - 1/n$ as in the closed-form of the van Genuchten model. Compressibility (Mv) is assumed 1×10^{-5} kPa^{-1} [6.9×10^{-5} psi^{-1}]. The hydraulic initial condition within the experimental column is given as a uniform volumetric water content of 0.35, which is equivalent to a pore water pressure of −43.33 kPa [−90.4 psi] using van Genuchten's (1980) analytical model. As such, the material activation pore water pressure will be set to −43.33 kPa [−90.4 psi] for both layers. The material properties of the surface layer do not differ from those of the nonsurface layer for this test case.

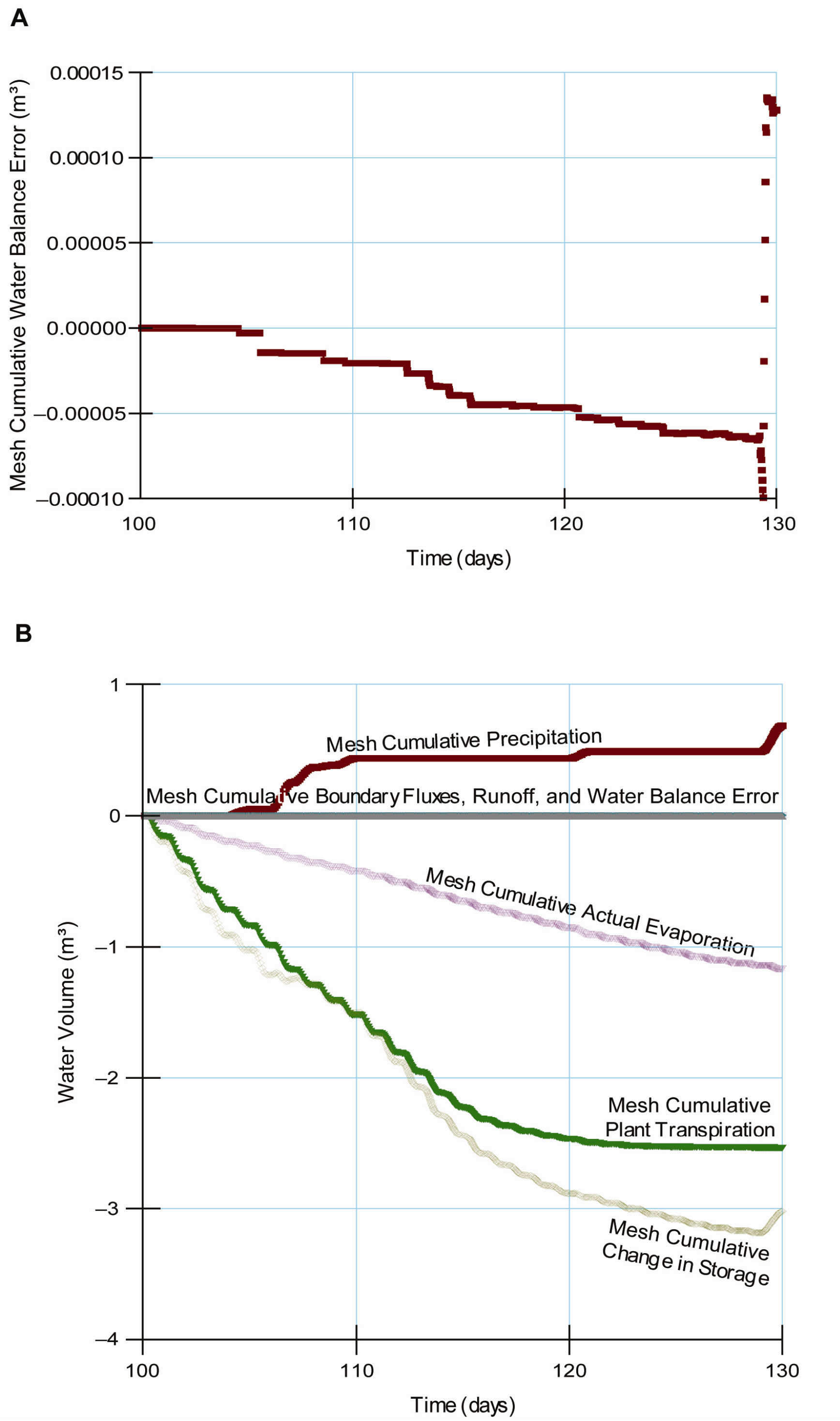

Figure 6. Test Case 2: Volumetric Water Balance: (A) Mesh Cumulative Water Balance Error and (B) Constituent Parts of the Volumetric Water Balance (Note That Mesh Cumulative Boundary Fluxes, Mesh Cumulative Runoff, and Mesh Cumulative Water Balance Error All Appear To Plot on the 0 m^3 Line at This Scale)

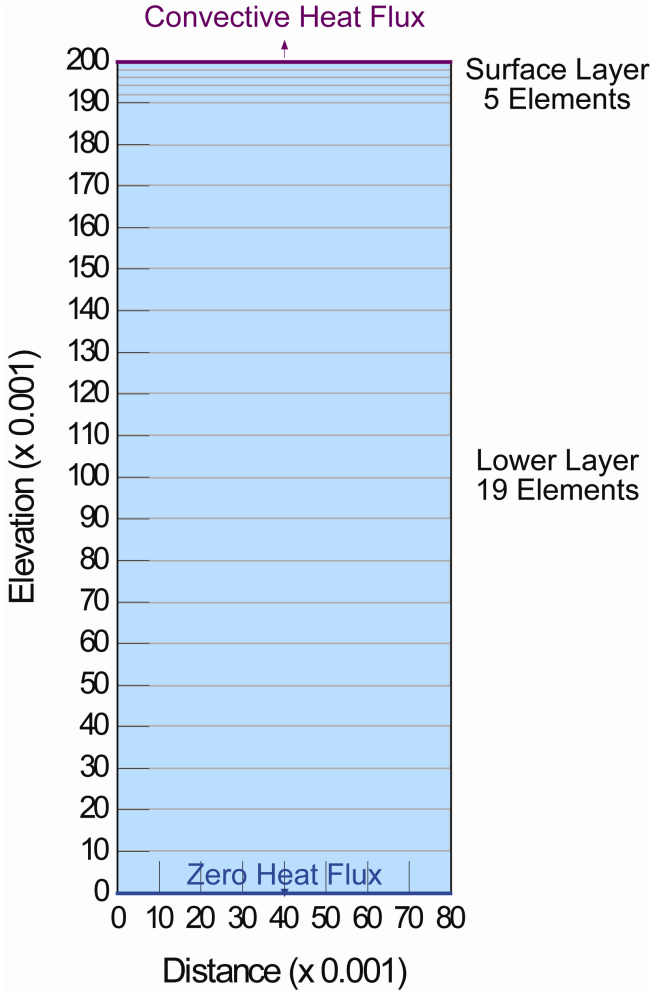

Figure 7. Rectangular Grid of Finite Element Quadrilaterals VADOSE/W Used in the Implementation of Test Case 3

This simulation uses a full thermal model with thermal conductivity data for Kanagawa sandy loam soil Mizoguchi (1990) measured as a function of water content and Hansson, et al. (2004, Figure 2, lower graph) documented. The thermal conductivity function assigned to both material layers is as shown in Figure 8A. The volumetric heat capacity function (Figure 8B) was estimated in VADOSE/W using the aforementioned soil moisture function and the de Vries (1975, 1963) method. The soil moisture function is used to determine the range of possible water contents over which the volumetric heat capacity function is defined. Mass specific heat of the soil minerals was assumed to be 0.71 J/g·°C [1.70×10^{-4} Btu/lb_m·°F] as given in GEO-SLOPE International, Ltd. (2007, Table 4-2). The thermal initial condition within the experimental column was given as a uniform temperature of 6.7 °C [44 °F]. As such, the material activation temperature will be set to 6.7 °C [44 °F].

The lower boundary conditions are zero water and zero heat flux. The upper boundary conditions are zero water flux and convective heat transfer modeled as

$$q_h = h_c \left[T_{Top} - T_{Coolant} \right] \tag{3}$$

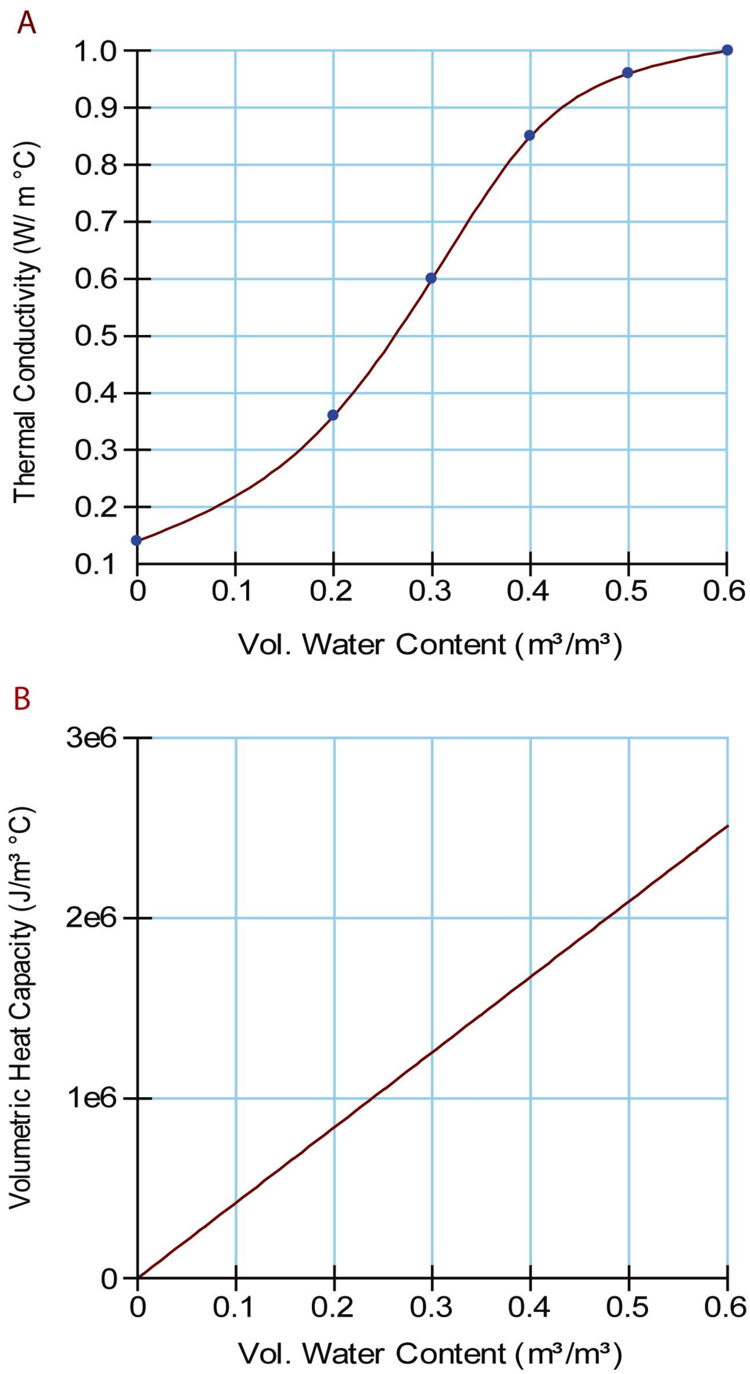

Figure 8. Full Thermal Model Functions for Test Case 3: (A) Spline Data Point Function for Measured Thermal Conductivity of Kanagawa Sandy Loam Soil Versus Unfrozen Volumetric Water Content (cf., Hansson, et al., 2004, Figure 2)
[1 $W \cdot m^{-1} \cdot °C^{-1}$ = 0.57782 $Btu \cdot hr^{-1} \cdot ft^{-1} \cdot °F^{-1}$];
(B) VADOSE/W Estimated Volumetric Heat Capacity Function
[1 $kJ \cdot m^{-3} \cdot °C^{-1}$ = 0.01496 $Btu \cdot ft^{-3} \cdot °F^{-1}$]

where

q_h	—	heat flux ($W{\cdot}m^{-2}$)
h_c	—	convective heat transfer coefficient = 28 $W{\cdot}m^{-2}{\cdot}K^{-1}$ [4.9 $Btu/h{\cdot}ft^2{\cdot}°F$]
T_{Top}	—	temperature at the soil surface (°C)
$T_{Coolant}$	—	temperature of the circulating fluid = −6 °C [21.2 °F]

5.3.1 Test Procedure

1. For matric suction in the range 0.0981 to 1,000,000 kPa [0.014 to 145,000 psi], calculate volumetric water content using the method of van Genuchten (1980) and the model parameters Ishida (1983) determined without setting $m = 1 - 1/n$ in the spreadsheet file named *Hansson et al. 2004.xls*.

2. In VADOSE/W: Set units and scale; draw model geometry; specify material properties (including initial conditions) and boundary conditions; mesh model domain; establish adaptive timestepping. To specify the material properties for the soil moisture curve, create a data point function by copying the spreadsheet data created in Step 1 into the VADOSE/W Keyin Volumetric Water Content Functions window. To specify the convective heat transfer boundary condition, use a combination of the "*q*" boundary condition function and the Modifier function to create the convective heat transfer boundary condition.

3. Run VADOSE/W simulations for 180,000 seconds (50 hours).

4. Digitize measured values of total volumetric water content presented in Hansson, et al. (2004, Figure 4) for 12, 24, and 50 hours after freezing began.

5. Compare simulated and measured values of the total volumetric water content 12, 24, and 50 hours after freezing started.

5.3.2 Results

If VADOSE/W is capable of simulating water redistribution at a freezing front, the VADOSE/W simulations should agree with measured values of total volumetric water content within ±10 percent.

The simulation for Test Case 3 was performed on June 9, 2008. Numerical results are contained in VADOSE/W file *Hansson et al. 2004.gsz* and are compared with measured laboratory data in Microsoft Excel file *Hansson et al. 2004.xls* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008). The VADOSE/W results (Figure 9) indicate VADOSE/W does not currently have the capability to model moisture redistribution toward a freezing front through cryogenic suction (or moisture redistribution away from a thawing interface). While it is likely that VADOSE/W was able to approximate the temperature distribution of the Mizoguchi (1990) laboratory experiment, Hansson, et al. (2004) did not provide the measured temperature distribution, and thus the experimental results cannot be compared against model results. Communication with Greg Newman,[1] VADOSE/W author,

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[1] Newman, G. "Question on Material Properties Not Solved Accurately by Test Case 3." Email (June 10) to C. Dinwiddie, Geosciences and Engineering Division, Southwest Research Institute®. Calgary, Alberta, Canada: GEO-SLOPE International, Ltd. 2008.

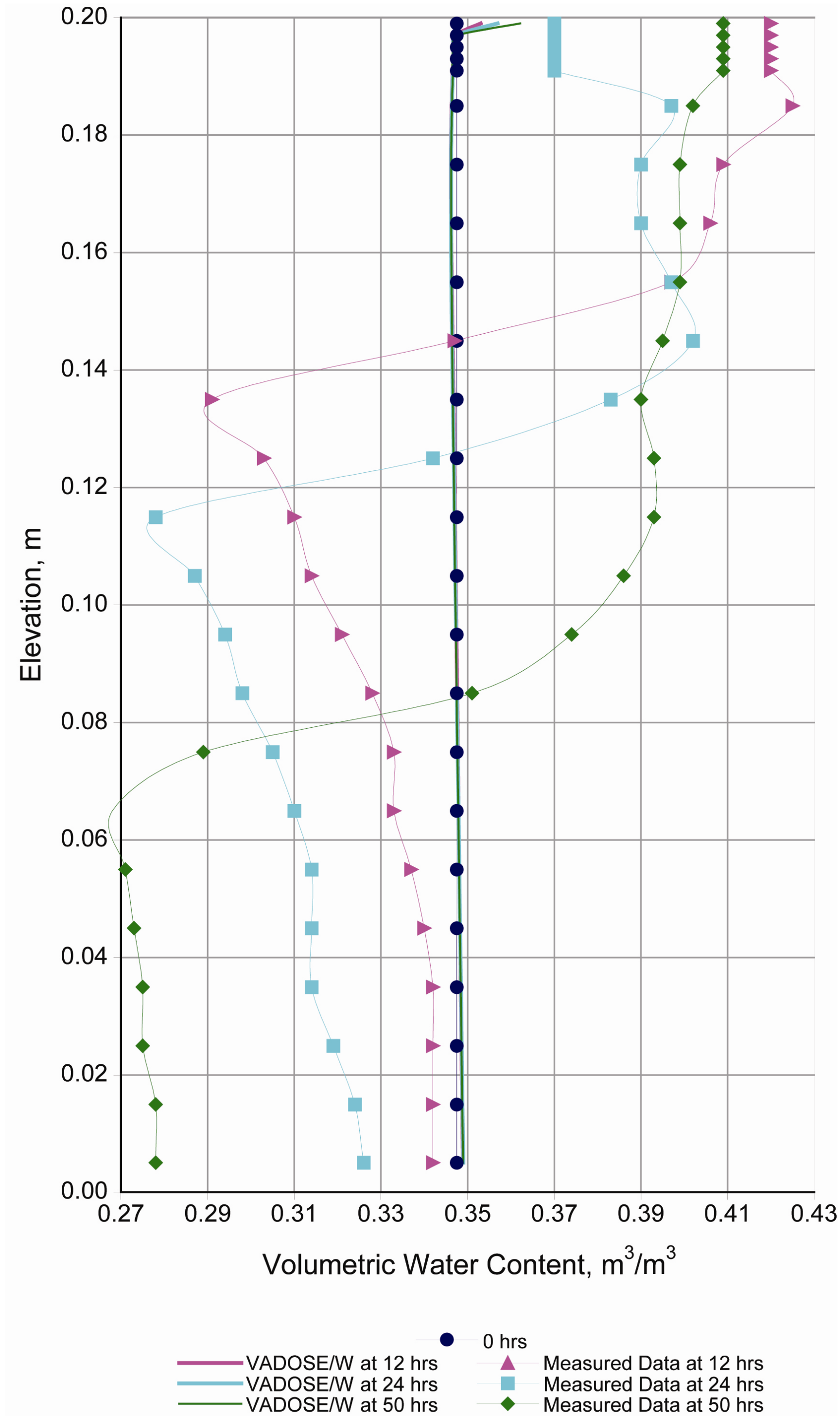

Figure 9. Test Case 3: Comparison of Volumetric Water Content as a Function of Elevation and Time as Measured by Mizoguchi (1990) and Computed by VADOSE/W. The VADOSE/W Results Show No Water Redistribution in the Modeled Soil Column as a Function of Time, Indicating VADOSE/W Is Not Capable of Simulating This Laboratory Experiment.

confirmed that VADOSE/W cannot replicate the laboratory experimental results of Mizoguchi (1990). The heat and mass transfer equations in the current version of VADOSE/W are coupled by vapor flow, but not by a cryogenic suction term. Newman indicated that if water migration to a freezing front (typically limited in clay soil covers) is neglected, VADOSE/W can typically match within reason any freezing/thawing/phase change simulation or lab study. VADOSE/W models ground freezing accurately only when it is appropriate to assume that water movement to an advancing freezing front is insignificant. In many engineered cover systems, this is an appropriate assumption because the amount of water present is limited and the only saturated material is often low hydraulic conductivity clay wherein significant amounts of flow would not be expected. Newman further explained that

> "In a ground freezing model where you are interested in the depth of frost penetration over a 6 to 8 foot depth range, the assumption that water does not move [to] the frost front due to "suction" may make a half foot difference. In a 20 cm column in a lab, it will make a big difference. In an artificial ground freezing model where brine is circulated in pipes [see Test Case 6, for example] to create frozen barrier walls, no one considers cryogenic suction an issue and in fact most don't even consider flowing water an issue. The importance of cryogenic suction depends greatly on the availability of a water source, the conductivity (hydraulic) of the material, and the duration of freezing.
>
> "In VADOSE[/W], the assumption that there is no cryogenic suction will affect all of the parameters...Ice, water, unfrozen water, air, and saturation are all directly tied to the amount of water moving in the system. They also affect the thermal properties and therefore the temperature profile and location of freezing front. I said…earlier…that the temperature profile would likely be close to Hansson [et al., 2004] but this is just based on my experience with very small scale samples undergoing freezing where there are strict controls on boundary temperatures at the warm and cold ends of the sample. In this type of setting, heat conduction tends to dominate the process and small changes in ice/water content don't have a huge impact on temperature profiles.
>
> "If you modeled a low conductivity clay material then VADOSE[/W] would do extremely well at predicting all of the parameters... If you model a high conductivity sand with a source of water near it, VADOSE[/W] would start to diverge from the real processes occurring in the soil."

Because VADOSE/W failed this validation test, three additional test cases that investigate the software capabilities for handling freezing and thawing phase change processes are documented next. Although VADOSE/W failed this validation test, the results of the two-dimensional Test Case 6, discussed later, indicate that VADOSE/W can simulate phase change on a field scale.

5.4 Test Case 4: Simulation of Phase Change Under Freezing Conditions

Test Case 4 simulates the advance of a freezing front within a column of water and compares the numerical solution with the freeze depth computed using the Neumann analytical solution. The solution for the advance of a freezing front that Neumann developed circa 1860 is given by the Neumann equation presented in Carslaw and Jaeger (1947)

$$X = \alpha\sqrt{t} \tag{4}$$

where

X	—	depth of freezing (or thawing) front [m]
α	—	constant parameter based on material properties and boundary conditions [m·days$^{-½}$]
t	—	elapsed time [days]

Nixon and McRoberts (1973) prepared the Neumann equation graphical solution shown in Figure 10. In summary, this chart indicates

$$\frac{\alpha}{2\sqrt{k_u}} = f\left\{Ste,\ -\frac{T_g K_f}{T_s K_u}\left(\frac{k_u}{k_f}\right)^{1/2}\right\} \tag{5}$$

where

k_u	—	unfrozen material diffusivity = K_u/C_u [m^2/day]
k_f	—	frozen material diffusivity = K_f/C_f [m^2/day]
K_u	—	unfrozen material thermal conductivity [kJ/day·m·°C]
K_f	—	frozen material thermal conductivity [kJ/day·m·°C]
C_u	—	unfrozen material volumetric heat capacity [kJ/m^3·°C]
C_f	—	frozen material volumetric heat capacity [kJ/m^3·°C]
Ste	—	Stefan no. = $C_u \cdot T_s / L$ [dimensionless]
L	—	volumetric latent heat [kJ/m^3]
T_g	—	uniform initial temperature [°C]
T_s	—	step change in temperature [°C] applied at the surface at t = 0 days

The analytical solution is one for a column of water undergoing freezing with the parameters and conditions specified in Figure 11. Because $k_u = k_f$ and $K_u = K_f$ is assumed for simplicity, the second parameter in the Eq. (5) function simply reduces to $-T_g/T_s = -(3\ °C/-5\ °C) = 0.6$. The dimensionless Stefan no. is (2,000 kJ/m^3·°C)(−5°C)/(−334,000 kJ/m^3) = 0.03. Using these two variables, one enters Figure 10 at Ste = 0.03, moves up to the curve labeled 0.6, and left to the normalized parameter axis at a value of 0.12. The parameter α is then calculated to be 0.12(2)√(100/2,000) = 0.054 m·days$^{-½}$ [0.18 ft·days$^{-½}$].

Simulations are performed using a simplified thermal model for a column of water with the parameters specified in Figure 11. The thermal initial condition within the water column will require the material activation temperature to be set to 3 °C [37.4 °F], and the upper and lower thermal boundary conditions are as shown in Figure 11.

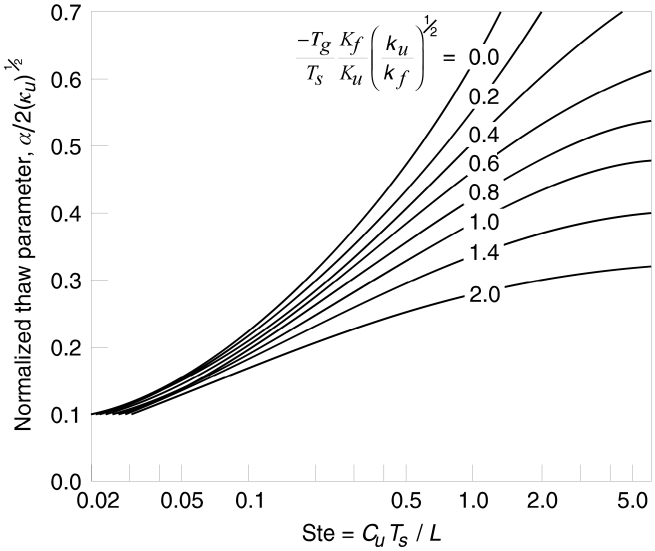

Figure 10. Graphical Solution of the Neumann Equation [Reproduced From GEO-SLOPE's *Freeze Column Examples.pdf* With Permission; After Nixon and McRoberts (1973)]

VADOSE/W simulations for this transient, one-dimensional test case use a 5-m-high by 1-m-wide [16.4-ft-high by 3.2-ft-wide] rectangular grid of finite element quadrilaterals. A surface layer was not used for this test case. For ease of locating the position of the unfrozen/frozen interface as a function of time, the mesh consists of 1 element in the horizontal direction and 600 elements in the vertical direction, and thus, due to element density, the test case mesh is not shown in Figure 11.

Because the simulation is of a freezing column of water in the absence of soil minerals, the volumetric water content is 1 m^3/m^3 [1 ft^3/ft^3], and the hydraulic "material properties" will be specified stylistically for an essentially fully saturated "clay" with large saturated hydraulic conductivity {1,000 m/d [3,281 ft/d]} and elevated residual moisture content {0.99 m^3/m^3 [0.99 ft^3/ft^3]}. The compressibility (*Mv*) of water was assumed 0 kPa^{-1} [0 psi^{-1}]. The material activation pore water pressure will be set to 0.01 kPa [1.45×10^{-3} psi].

5.4.1 Test Procedure

1. In VADOSE/W: Set units and scale; draw model geometry; specify material properties (including initial conditions) and boundary conditions; mesh model domain.

2. Run VADOSE/W simulations for 1,182 days.

3. Output numerical results for the temperature distribution in the water column to spreadsheet file *Freezing Column Temperature Data.xls*. Identify the unfrozen/frozen interface {where T = 0 °C [32 °F]} as a function of time.

4. Calculate depth of freezing front analytically using Eq. (4) and the procedure identified above in spreadsheet file *Freezing Column Temperature Data.xls*. Compare numerical and analytical values of the freeze depth as a function of time after the step change in surface temperature.

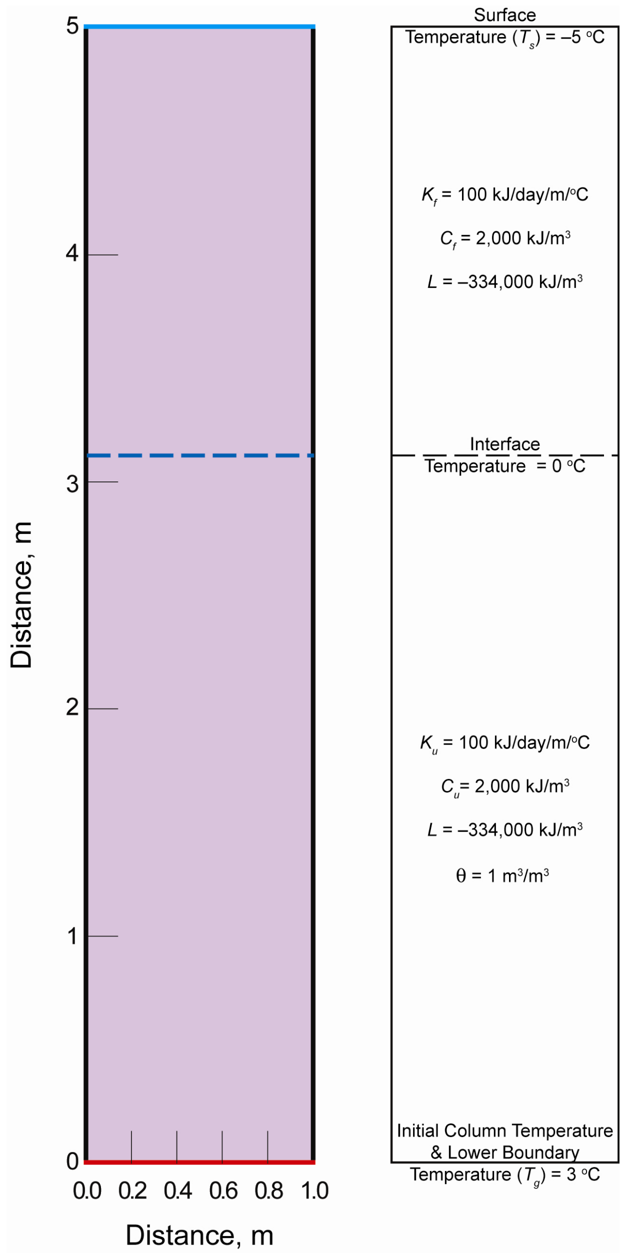

Figure 11. Test Case 4: Geometry and Problem Statement

5.4.2 Results

The VADOSE/W simulations should agree with calculations using Figure 10 and Eq. (4) within ±10 percent.

The simulations for Test Case 4 were performed on July 24, 2008. Analytical and numerical results are contained in Microsoft Excel file *Freezing Column Temperature Data.xls* and VADOSE/W file *Nixon and McRoberts 1973.gsz* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008).

The comparisons between the temperature distribution VADOSE/W computed as a function of time and location of the freezing front computed using the Neumann analytical solution are shown in Figure 12. The VADOSE/W results agree with the Neumann analytical solution within 9.7 percent. The results of this validation test are acceptable.

5.5 Test Case 5: Simulation of Phase Change Under Thawing Conditions

Test Case 5 simulates essentially the reverse process modeled in Test Case 4 with the same geometry but different material properties and boundary conditions. Equations (4) and (5) are still relevant, as is Figure 10, and their development is not repeated here. The problem is defined as a column undergoing thawing with the material properties (Figure 13) defined in Hwang, et al. (1972) when they tested their numerical model against the Neumann solution.

Again, for simplicity Hwang, et al., (1972) defined, $k_u = k_f$ and $K_u = K_f$, so the second parameter in the Eq. (5) function simply reduces to $-T_g/T_s = -(-2\ °C/5\ °C) = 0.4$. The dimensionless Stefan no. is (4186.8 kJ/m^3·°C)(5°C)/(209,340 kJ/m^3) = 0.1. Using these two variables, one enters Figure 10 at Ste = 0.1, moves up to the curve labeled 0.4, and left to the normalized parameter axis at a value of 0.2. The parameter α is then calculated to be 0.2(2)√(100/4186.8) = 0.062 m·days$^{-½}$ [0.20 ft·days$^{-½}$].

Simulations are performed using a simplified thermal model for a column with the parameters specified in Figure 13. The thermal initial condition within the column will require the material activation temperature to be set to −2 °C [28.4 °F], and the upper and lower thermal boundary conditions are as shown in Figure 13. VADOSE/W simulations for this transient,

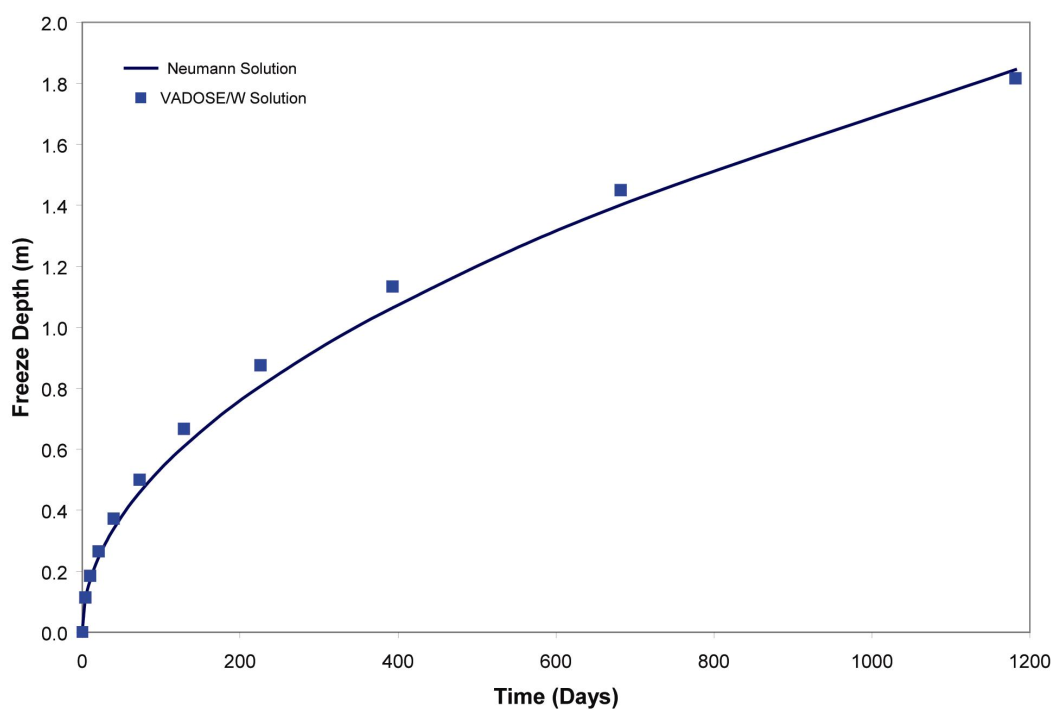

Figure 12. Test Case 4: Comparison of Freeze Depth as a Function of Time Following a Step Change in Surface Temperature Using VADOSE/W and the Neumann Analytical Solution

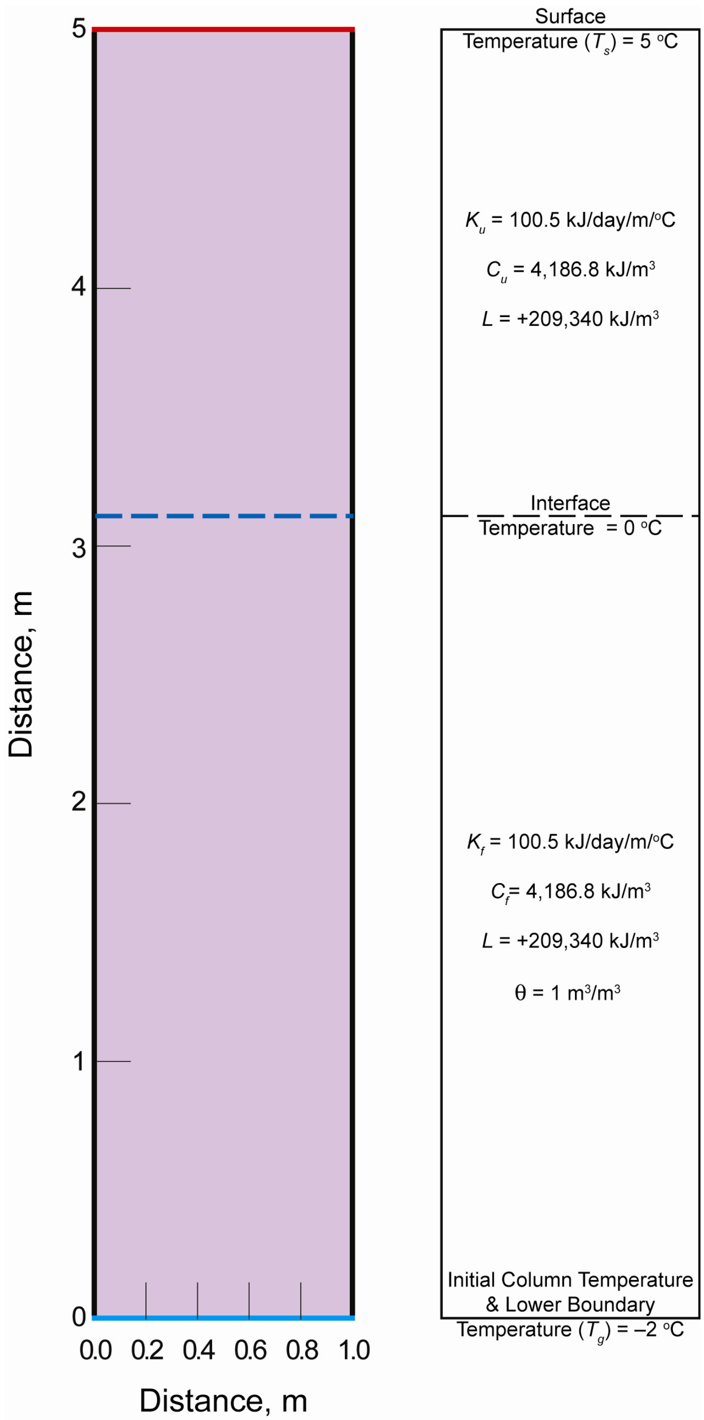

Figure 13. Test Case 5: Geometry and Problem Statement

one-dimensional test case will use the same geometry and same element mesh as used for Test Case 4 (Figure 13). The hydraulic “material properties” will also be specified in the same manner as for Test Case 4.

5.5.1 Test Procedure

1. In VADOSE/W: Create a copy of the Test Case 4 VADOSE/W file and rename it because the Test Case 4 geometry will be used for Test Case 5. Input a revised latent heat consistent with that Hwang, et al. (1972) used. Specify new thermal material properties (including initial conditions) and boundary conditions consistent with those Hwang, et al. (1972) used.

2. Run VADOSE/W simulations for 263 days, and output the temperature distribution solutions at 1, 66, and 263 days, consistent with Hwang, et al. (1972, Figure 2).

3. Copy numerical results for the temperature distribution in the column to spreadsheet file *Thawing Column Temperature Data.xls*. Identify the unfrozen/frozen interface {where T = 0 °C [32 °F]} as a function of time.

4. Calculate depth of thawing front analytically using Eq. (4) in spreadsheet file *Thawing Column Temperature Data.xls*. Compare numerical and analytical values of the thaw depth as a function of time after the step change in surface temperature. Calculate percent difference between numerical and analytical results in spreadsheet file *Thawing Column Temperature Data.xls*.

5.5.2 Results

The VADOSE/W simulations should agree with calculations using Figure 10 and Eq. (4) within ±10 percent.

The simulations for Test Case 5 were performed on July 25, 2008. Analytical and numerical results are contained in Microsoft Excel file *Thawing Column Temperature Data.xls* and VADOSE/W file *Hwang et al. 1972.gsz* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008).

The comparisons between the temperature distribution VADOSE/W computed as a function of time and location of the thawing front computed using the Neumann analytical solution are shown in Figure 14. The VADOSE/W results agree with the Neumann analytical solution within 9.9 percent. The results of this validation test are acceptable.

5.6 Test Case 6: Simulation of Frost Bulb Development Around a Buried Pipeline

Test Case 6 simulates development of a frost bulb around a buried freeze pipe and compares the VADOSE/W result with what Coutts and Konrad (1994) obtained when they simulated the same system with their finite element node state method. This test case, which models artificial ground freezing used to create frozen containment barrier walls, was undertaken to validate the phase change capabilities of VADOSE/W at field scale with a two-dimensional simulation.

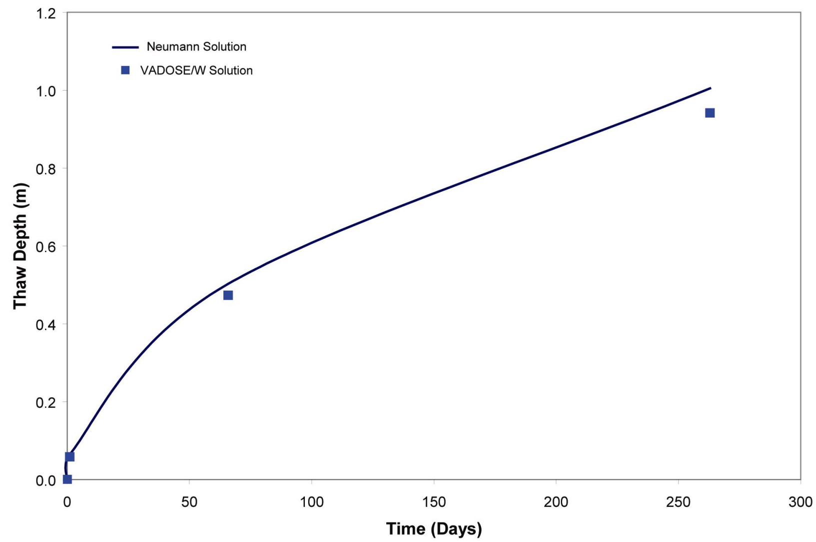

Figure 14. Test Case 5: Comparison of Thaw Depth as a Function of Time Following a Step Change in Surface Temperature Using VADOSE/W and the Neumann Analytical Solution

The model and mesh geometry is as shown in Figure 15, which illustrates a cross section of a freeze pipe buried 0.3 m [0.98 ft] below ground. Before the freeze pipe begins operation, the ground temperature is 3 °C [37.4 °F], so this value will be applied as the material activation temperature initial condition within the model domain and also as the ground surface boundary condition. The boundary condition on the freeze pipe after $t = 0$ is −2 °C [28.4 °F]. The far field and line of symmetry thermal boundary conditions will implicitly be no heat flux.

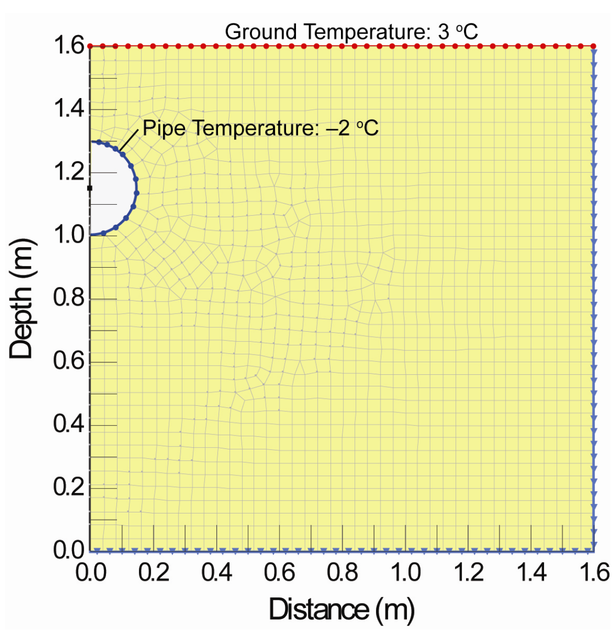

Figure 15. Model Geometry and Unstructured Quadrilateral and Triangle Element Mesh VADOSE/W Used in the Implementation of Test Case 6

Simulations will be performed using a simplified thermal model. The frozen soil thermal conductivity will be set to 155.52 kJ/d·m·°C [1.0401 Btu/h·ft·°F], and the unfrozen soil thermal conductivity will be set to 129.6 kJ/d·m·°C [0.8667 Btu/h·ft·°F]. The volumetric heat capacity for both frozen and unfrozen soil will be set to 1950 kJ/m^3·°C [29.07 Btu/ft^3·°F].

Coutts and Konrad (1994) specified the latent heat of the selected soil as 126,000 kJ/m^3·°C [4,230 Btu/ft^3·°F], so the volumetric water content is calculated as the latent heat of soil 126,000 kJ/m^3·°C [4,230 Btu/ft^3·°F] divided by the latent heat of water 334,000 kJ/m^3·°C [1,590 Btu/ft^3·°F], equal to 0.3772 m^3/m^3 [0.3772 ft^3/ft^3]. The volumetric water content function will thus be estimated using a VADOSE/W sample function for clay with saturated water content 0.3772 m^3/m^3 [0.3772 ft^3/ft^3], and the material activation pore water pressure initial condition will be set to 0.01 kPa [1.4×10^{-3} psi]. The compressibility (*Mv*) is assumed at 0 kPa^{-1} [0 psi^{-1}]. The hydraulic boundary condition at the ground surface will be set at a pressure head of 1 m [3.281 ft]; the far field and line of symmetry hydraulic boundary conditions will implicitly be no flow.

5.6.1 Test Procedure

1. In VADOSE/W: Set units and scale; draw model geometry; specify material properties (including thermal and hydraulic initial conditions) and boundary conditions; mesh model domain.

2. Run VADOSE/W simulation for 730 days [2 yr].

3. Graph the temperature distribution at the end of 2 years, and compare to the temperature distribution Coutts and Konrad (1994) obtained. Calculate percent difference between the VADOSE/W and Coutts and Konrad (1994) model results for the lateral and vertical extent of the frost bulb as measured from the pipe surface.

5.6.2 Results

The VADOSE/W simulated position of the freezing front relative to the side and bottom of the pipe should agree within ±5 percent with the position Coutts and Konrad (1994) determined using their node state finite element model of the same problem.

The simulation for Test Case 6 was performed on July 25, 2008. Numerical results are contained in VADOSE/W file *Coutts and Konrad 1994.gsz* on the VADOSE/W validation CD associated with Scientific Notebook 933E (Dinwiddie, 2008).

Coutts and Konrad (1994) show that the frost bulb {interface at T = 0 °C [32 °F]} extends 0.60 m [2 ft] below and 0.23 m [0.75 ft] horizontally to the side of the pipe at the end of 2 years. The comparison between the temperature distribution Coutts and Konrad (1994) computed and that computed by VADOSE/W is shown in Figure 16. The VADOSE/W results are virtually identical to the Coutts and Konrad (1994) results (Figure 16); agreement is within 5 percent. The results of this validation test are acceptable.

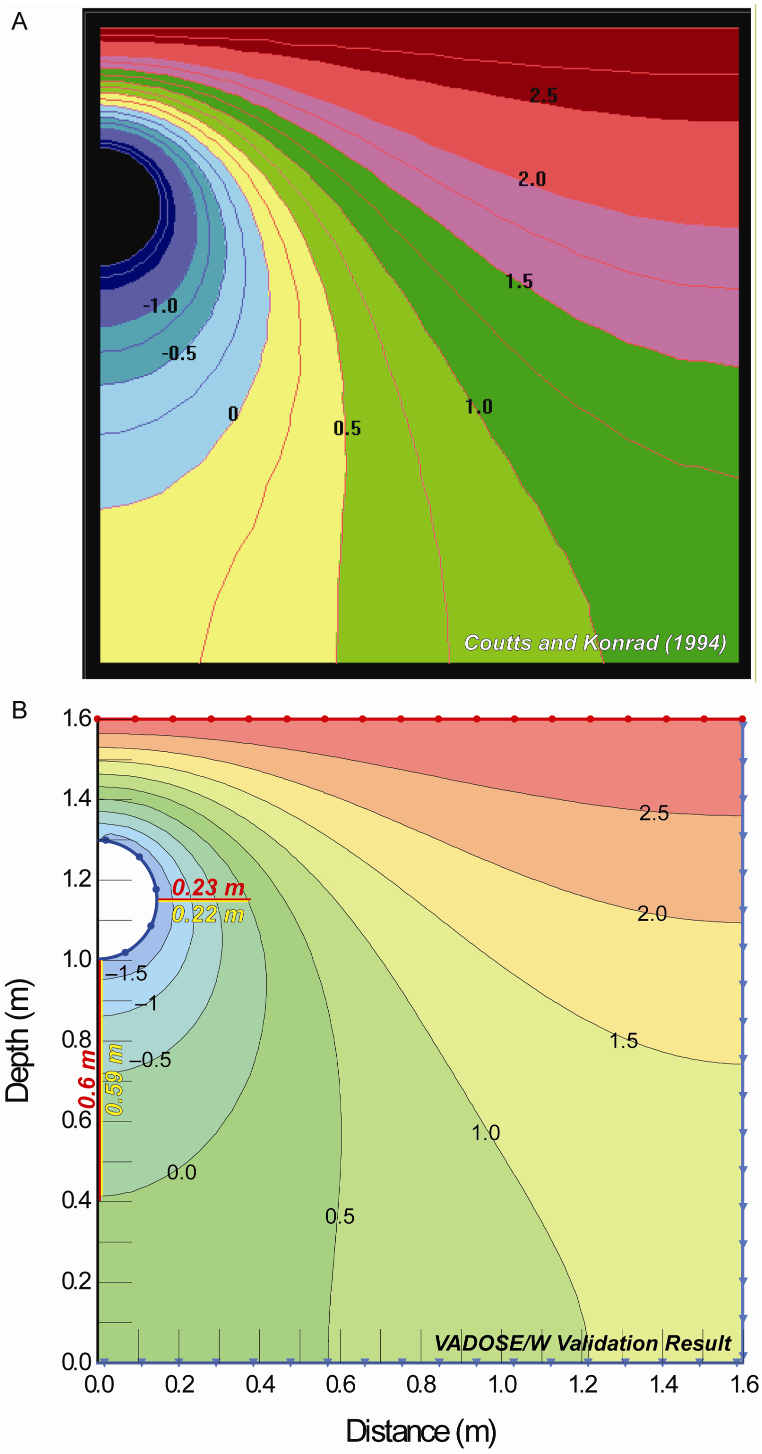

Figure 16. Test Case 6: Temperature Distribution Around a Buried Freeze Pipe at Time *t* = 730 days [2 yr]. (A) Coutts and Konrad (1994) Found the Frost Bulb Extends 0.6 m [1.97 ft] Below the Pipe and 0.23 m [0.75 ft] to the Right of the Pipe (Reproduced From GEO-SLOPE's *Pipeline Freezing Analysis.pdf* With Permission); (B) In Comparison, VADOSE/W Determined the Frost Bulb Extends 0.59 m [1.94 ft] Below the Pipe and 0.22 m [0.72 ft] to the Right of the Pipe.

6 CONCLUSIONS

Many of the most important functionalities of VADOSE/W (Table 1) were tested through this software validation activity and found to produce acceptable results. The scope of the validation is therefore limited to those functionalities that were successfully tested. Test Case 3 showed that VADOSE/W is not currently coded for modeling water migration as a function of cryosuction; however, this process may not always be important, and this capability may be added to VADOSE/W in the future, per communication with Greg Newman[2] of GEO-SLOPE. Snow accumulation, melt, and ablation functionalities were not tested as part of this software validation. Despite some remaining questions regarding the implementation and documentation of the snow accumulation, melt, and ablation algorithms in VADOSE/W, the software validation performed indicates that VADOSE/W is a suitable code for evaluating infiltration and percolation through engineered soil covers, including the Ronald W. Reagan National Defense Authorization Act of Fiscal Year 2005 (NDAA) soil covers. VADOSE/W should be useful for modeling the flow of water associated with NDAA soil covers, including movement of fluids to embedded drains, and infiltration of water into waste and lower lying regions. A published validation study of VADOSE/W (Adu-Wasu, et al., 2007) included a simulation of a geosynthetic clay liner membrane. VADOSE/W can simulate geo-fabrics using free line geometry objects (Walter and Dubreuilh, 2007) that can be assigned material and interface models. This specific application was not tested via this software validation report. In addition, none of the test cases resulted in surface ponding and redistribution of runoff, although this capability of the code was active. Site-specific application of VADOSE/W could result in ponding and runoff, in which case the user should verify that a water mass balance is preserved. While not every functionality of VADOSE/W was tested herein, the result of this software validation is that the functionalities of VADOSE/W addressed in Test Cases 1, 2, 4, 5, and 6 (Table 1) are fully validated. The software is thus released for general use, and specifically for regulatory review and oversight purposes.

For modeling the vadose zone hydrology related to NDAA tank closures in Washington, Idaho, and New York, one must consider whether it is important to model water migration toward a freezing front. On a case-by-case basis, staff should consider whether cryosuction and snow accumulation, melt, and ablation are important processes that must be modeled accurately. In many cases, it may be enough to simply have frozen interstitial water and any snow act as aqueous reservoirs that are activated during spring thaw each year. If it is sufficient for the model to simply accumulate and store precipitation during the winter months and release this stored moisture during spring thaw, the inability to specifically model the cryosuction process may not be particularly limiting.

VADOSE/W is not an engineered soil cover degradation model. It cannot be used to model erosion or biointrusion (although VADOSE/W can, however, model the hydrological processes associated with plant transpiration and the hydraulic effects of bioturbation when appropriate material properties can be defined). To model the hydrological processes associated with a degrading soil cover, one might iterate between the time-dependent topographies that produce landscape evolution models like SIBERIA (Willgoose, 2005) and CHILD (Tucker, et al., 1999) and resultant hydrological effects using a code such as VADOSE/W.

VADOSE/W should be among the first codes considered for modeling vadose zone and saturated zone hydrological processes in two dimensions at NDAA sites. The code features a

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[2]Newman, G. "Adding Cryogenics to VADOSE/W." Email (June 9) to C. Dinwiddie, Geosciences and Engineering Division, Southwest Research Institute. Calgary, Alberta, Canada: GEO-SLOPE International, Ltd. 2008.

relatively easy-to-use Windows-based graphical user interface that facilitates the development of physically based hydrological models of soil cover processes.

APPENDIX A

This appendix provides additional background to support the selected validation test cases by presenting an excerpt from our preliminary evaluation of VADOSE/W in its original format. The preliminary evaluation was transmitted to NRC on April 25, 2008.[1]

In recent years, a number of soil cover numerical studies have been published in the literature (Fayer, et al., 1992; Fayer and Gee, 1997; Khire, et al., 1999, 1997; Scanlon, et al., 2005, 2002; Benson, et al., 2005, 2004; Ogorzalek, et al., in press). Bohnhoff, et al. (in press) evaluated four codes for simulating soil covers using test site data from a water balance cover site in Altamont, California (Benson, et al., 2001, 1999; Albright, et al., 2004); VADOSE/W v. 6.02 (not VADOSE/W 2007) was among the evaluated codes. We evaluated whether the data and modeling reported in this unpublished paper may form the basis of a future validation study for VADOSE/W. We concluded that any experimental study tests some, but not all of the functionalities of VADOSE/W. For example, the Bohnhoff, et al. (in press) study is only relevant to one-dimensional water flow and heat transfer with unit gradient and seepage face lower boundary conditions (processes other than water flow and heat transfer were not addressed via data collection). Furthermore, while the Journal of Geotechnical and Geoenvironmental Engineering (ASCE) has accepted this paper for publishing (expected within 6 months) (C.H. Benson, personal communication, April 2008), not all data used in the Bohnhoff, et al. (in press) study are available in the unpublished journal article (e.g., the detailed meteorological data associated with the test site over the three-year duration of data collection is lacking). Therefore, to pursue this validation study, unpublished meteorological data would need to be secured from these authors or else data published elsewhere (perhaps in Ogorzalek, 2005) would have to be obtained and used as model input.

Experimental field studies that are documented in the professional literature, such as those noted previously, are often plagued with ill-defined data uncertainties—particularly in the soil hydraulic properties and atmospheric boundary conditions; these uncertainties make comparison between experimental data and modeling results difficult to perform and evaluate. While the principles governing aqueous flow and heat transfer are well established, we need to validate that VADOSE/W 2007 properly solves these problems. This validation can be performed by comparing modeling results with established analytical solutions or validated codes, which is the approach specified in CNWRA [Center for Nuclear Waste Regulatory Analyses] Technical Operating Procedure (TOP)–18.

The major functionalities of the code should be validated in a risk-informed manner if their use is anticipated during regulatory review—testing the major functionalities of the code will likely require several small numerical experiments. Validating the snow accumulation and ablation algorithm and the soil freeze–thaw algorithm should be emphasized. Because no other numerical modeling codes with these functionalities have been validated according to TOP–18, the freezing soil algorithm and the snow accumulation and ablation algorithm will need to be

[1]Walter, G. "Preliminary Evaluation of VADOSE/W." Email (April 25) to M. Fuller, U.S. Nuclear Regulatory Commission. San Antonio, Texas: Geosciences and Engineering Division, Southwest Research Institute®.

validated using experimental data. Hansson, et al. (2004) presented one such study of soil freezing in a vertical laboratory column [after work performed by Mizoguchi (1990)]; this study will likely be amenable for validating the soil freezing algorithm of VADOSE/W 2007. Finally, the validation should emphasize the deftness with which the code handles the atmospheric boundary, ponding, and runoff. This might be accomplished by evaluating the mass balance.

With respect to meeting CNWRA quality assurance requirements, the validation effort should focus on (i) verifying that VADOSE/W correctly solves the fundamental equations and constitutive relationships governing unsaturated water flow, (ii) verifying that VADOSE/W correctly handles atmospheric and ponding boundary conditions and maintains any acceptable mass balance, and (iii) testing the validation of certain approximations used in implementing frozen soil and snow accumulation and ablation process models.

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