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EVALUATION OF HELP MODEL REPLACEMENT CODES

Authors: **Tad Whiteside**
Thong Hang
Gregory Flach

JULY 2009

Savannah River National Laboratory
Savannah River Nuclear Solutions
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REVIEWS AND APPROVALS

3/19/2010

Tad S. Whiteside, Co-author, Environmental Science and Biotechnology — Date

4/26/2010

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3/19/2010

Gregory P. Flach, Co-author, Environmental Science and Biotechnology — Date

4/26/2010

Heather Burns, Manager, Radiological Performance Assessment — Date

Tom Robinson, Manager, Closure and Waste Disposal Assessment — Date

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LIST OF ACRONYMS

DOE	Department of Energy
HELP	Hydrologic Evaluation of Landfill Performance
USEPA	United States Environmental Protection Agency
USACE	Unites States Army Corps of Engineers
PA	Performance Assessment
WES	Waterways Experiment Station

ABSTRACT

This work evaluates the computer codes that are proposed to be used to predict percolation of water through the closure-cap and into the waste containment zone at the Department of Energy closure sites. This work compares the currently used water-balance code (HELP) with newly developed computer codes that use unsaturated flow (Richards' equation). It provides a literature review of the HELP model and the proposed codes, which result in two recommended codes for further evaluation: HYDRUS-2D3D and VADOSE/W. This further evaluation involved performing actual simulations on a simple model and comparing the results of those simulations to those obtained with the HELP code and the field data. From the results of this work, we conclude that the new codes perform nearly the same, although moving forward, we recommend HYDRUS-2D3D.

1.0 EXECUTIVE SUMMARY

Computer modeling is conducted to evaluate the long-term performance of closure caps and other waste-containment systems. The two primary methods used to analyze the performance of waste-containment covers are: (I) simplified water balance and (II) unsaturated flow. Both methods incorporate environmental variables to predict water flow through the waste-containment cover; however, each uses a different approach to account for percolation. The simplified water balance is the method currently used and the goal of this work is to evaluate the new codes that incorporate unsaturated flow as part of their modeling strategy.

As the first step in this evaluation, a literature review was undertaken to enumerate shortcoming of the currently used model (HELP) and to identify other candidate codes. From this literature analysis, we selected two codes, HYDRUS-2D3D and VADOSE/W, in addition to the HELP model, to evaluate.

The data requirements of these codes were evaluated and the necessary data sets were compiled.

Each of these codes was evaluated for stability, speed, and accuracy. Each code was used to solve a simple problem and the results were compared with those obtained with HELP and field measurements.

These models were analyzed based on the marginal costs and the marginal benefits of replacing the currently used system.

The conclusion was reached that either HYDRUS-2D3D or VADOSE/W are adequate for modeling the water-flow, but HYDUS-2D3D has benefits that outweigh those of VADOSE/W. More rigorous modeling of actual proposed cap systems must be carried out before a definite decision to replace HELP with HYDRUS-2D3D can be made.

2.0 INTRODUCTION

Computer modeling has been carried out since the early 1970's to evaluate the long-term performance of closure caps and other waste-containment systems. As computers have grown more powerful, it has become practical to develop more realistic models describing these systems. In the waste-containment realm, this means including the known environmental pathways for water flow. These pathways are affected by variables such as temperature, wind speed, relative humidity, solar radiation, soil composition, and plant types. The two primary methods used to analyze the performance of waste-containment covers are: (I) simplified water balance and (II) unsaturated flow (Zornberg 2007). Both methods incorporate the environmental variables to predict water flow through the waste-containment cover; however, each uses a different approach to account for percolation.

The simplified water balance method is the older method and uses the conservation of mass at the soil surface to estimate the percolation through the cover. This method assumes a soil layer is able to contain a maximum amount of water, based on its field capacity suction, versus the pull of gravity. The amount of percolation through the cover is calculated as the difference between the total moisture of the layers and moisture removed by evapotranspiration, lateral run-off, and the field capacity of the soil. The HELP (Hydrologic Evaluation of Landfill Performance) code is an example of water balance code that is currently used in the performance analysis of waste-containment systems (Zornberg 2007).

Unsaturated flow is the more modern method used to analyze the performance of waste-covers. This method incorporates solving Richards' equation (Eq. 1) for various surface boundary conditions (e.g. water infiltration, overland runoff, evaporation, and transpiration) and bottom boundary conditions (e.g. unit hydraulic gradient, and seepage faces). Richards' equation is a coupled, nonlinear parabolic equation, solved using finite differences or finite elements:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[K\left(K_{ij}^{A}\frac{\partial h}{\partial x_u} + K_{iz}^{A}\right)\right] - S \qquad \text{Equation 1}$$

where θ is the volumetric water content [L^3L^{-3}], h is the pressure head [L], S is a sink term [T^{-1}], x_i (i=1,2) are the spatial coordinates [L], t is time [T], K_{ij}^{A} are components of a dimensionless anisotropy tensor $\mathbf{K}^A$, and K is the unsaturated hydraulic conductivity function [LT^{-1}] given by:

$$K(h,x,y,z) = K_s(x,y,z)K_r(h,x,y,z) \qquad \text{Equation 2}$$

where K_r is the relative hydraulic conductivity and K_s is the saturated hydraulic conductivity [LT^{-1}]. (HYDRUS Technical Manual 2006). The relevant outputs from using these equations include the transient moisture redistribution and basal percolation (Zornberg 2007). LEACHM, UNSAT-H, HYDRUS-2D3D, and VADOSE/W are examples of codes that implement Richards' equation and are used to analyze evapotranspirative covers.

Although the codes incorporating Richards' equation are more sophisticated, it was unclear from the literature if using them would provide a tangible benefit to the prediction of the performance of waste-containment systems; specifically, would these codes more accurately describe the percolation of water through the closure caps and into the contaminated zone. Therefore, the objective of this study was to evaluate how these modern codes compare with the HELP model code, which is the current standard used in the Savannah River Site's waste-containment performance assessment process. The items being evaluated for each code are: the data requirements, the stability, the speed, and the accuracy - as compared to the HELP model. The results from this study will aid in determining if the benefits of using a new code outweigh the costs of switching and if they do, help determine which of these codes are most suited to meeting the needs of the Department of Energy's closure projects.

3.0 DISCUSSION

3.1 LITERATURE REVIEW

Of the two primary methods to analyze the performance of waste-containment covers, the simplified water balance method has been the preferred method for many years. This has been primarily due to a lack of model sophistication and computational power to run alternative codes. Recently, however, sophisticated models have been developed, which, with an increase of available computational power, has led stakeholders to ask for a corresponding increase in comprehensive modeling and a justification for the continued use of obsolete codes (NRC 2008). This work is in response to these comments and attempts to evaluate the available codes for applicability when used to analyze the performance of the proposed waste-containment systems.

As the first step in this evaluation, a literature review was undertaken to enumerate shortcoming of the currently used model (HELP) and to identify other candidate codes. From this literature analysis, we selected two codes, HYDRUS-2D3D and VADOSE/W, in addition to the HELP model, to evaluate.

There are various issues with selecting a code to use. This includes the difficulty of simulating some of the flow processes, e.g., runoff, ponding, etc (Piet 2003). Also, many of the available codes do not incorporate important processes, e.g., snow accumulation and melt, plant growth, etc. in their algorithms (Piet 2003). Further issues include the code development cycle: it usually falls into two categories: highly active development, with frequent changes or total abandonment. When a code is updated, it has to be revalidated, to ensure the update didn't change an essential component in an unexpected way, and this revalidation process is not simple, as the data input method may have changed between methods or new data is required. Some of the codes use parameters that are not easily measured or easily extracted from measured data. Also, the parameters' values may change over time (both with respect to the version of the model used and within the system being studied). Specific examples of these parameters include native vegetation transpiration properties and the hydraulic conductivity and water retention functions.

A similar review and evaluation of available codes was conducted by Benson and Shackelford (Shackelford 2006) from 2001-2006. They evaluated the hydrologic models:

LEACHM, UNSAT-H, HYDRUS-2D, and VADOSE/W using field data from five large-scale test facilities of alternative covers. Their work attempted to provide: (1) a baseline assessment and comparison of the algorithms in existing hydrologic models when applied to a variety of meteorological conditions; (2) an unbiased critical assessment of the predictive capabilities of existing hydrologic models for covers using field data from the EPA's Alternative Cover Assessment Program (ACAP); and (3) improvement of the hydrologic model (or models) that have the most promise so that predictions made with the model are accurate. Their study focused on comparing water-balance predictions for two alternative covers, a monolithic barrier and a capillary barrier, with the field measured water balance over three- and four-year periods. Water-balance predictions were obtained for both covers using LEACHM, HYDRUS-2D, and UNSAT-H, whereas VADOSE/W was included for the monolithic cover.

Their results showed that for the capillary barrier, all of the codes captured the seasonal variations in water-balance quantities observed in the field. They found that LEACHM and HYDRUS-2D predicted total runoff during the monitoring period with reasonable accuracy, but the timing of predicted versus observed runoff events was different; they found that UNSAT-H consistently over-predicted runoff. They found that all three codes predicted evapotranspiration reliably, when data from the first year were excluded. However, all three codes over-predicted evapotranspiration and under-predicted soil-water storage. This was primarily caused by late winter-early spring snowmelt which was not accounted for by the models during this time-frame. Predicted percolation was in good agreement with measured percolation, except during the first year. The problems with the first-year results imply that the models were not initialized properly (Shackelford 2006).

For the monolithic cover, the accuracy of the runoff prediction was found to affect the accuracy of all other water-balance quantities. Runoff was predicted more accurately when precipitation was applied uniformly throughout the day, the surface layer was assigned higher saturated hydraulic conductivity, or when Brooks-Corey functions were used to describe the hydraulic properties of the cover soils. They could not provide a definitive recommendation as to which of the above methods would provide reasonable assurance that runoff mechanisms are being properly simulated and the predictions are accurate. They found that the models predicted evapotranspiration and soil-water storage reasonably well - when runoff was predicted accurately, general mean hydraulic properties were used as input, and the vegetation followed a consistent seasonal transpiration cycle. However, they discovered that percolation was consistently under predicted even when evapotranspiration and soil-water storage were predicted reliably. They were able to obtain better agreement between measured and predicted percolation when the mean properties for the soil-water characteristic curve were used and the saturated hydraulic conductivity of the cover soils was increased by a factor between 5 and 10. Evapotranspiration and soil-water storage were predicted poorly at the end of the monitoring period by all of the codes due to a climate change that affected the evapotranspiration pattern and was not captured by the models. The inability to capture such changes was identified as a significant weakness in current modeling approaches and, therefore, as a need for future research (Shackelford 2006).
Benson and Shackelford's five-year review points out that each code has its own weakness and that the differences in predictions between models are greater than the differences due to

varying properties (Shackelford 2006, Benson 2007). These differences are usually caused by how the code handles the atmospheric boundary conditions. Other code features that have an impact on model results include: the initial conditions, the hydraulic properties model, hysteresis, vapor flow, thermally-driven flow, transpiration algorithms, ground freezing, snow melt, etc. Benson cautions that each of these features should be carefully considered so that realistic, but conservative results are obtained (Benson 2007).

The findings of Benson and Shackelford are consistent with Piet's results. Piet et al. examined four model codes (HYDRUS-2D, VADOSE/W, SWIM, and EDYS) and compared their results with HELP (Piet 2003). They concluded that only HYDRUS-2D and VADOSE/W are sufficient to model capillary barriers. From these and the following literature sources, we chose to focus this work on evaluating HYDRUS-2D3D and VADOSE/W.

The following sections describe the literature data available for the following codes: HELP, LEACHM, UNSAT-H, SVFlux, HYDRUS-2D3D, VADOSE/W.

3.1.1 HELP

The HELP model was developed by the United States Army Corps of Engineers (USACE) at the Waterways Experiment Station (WES) in Vicksburg, Mississippi under an interagency agreement (DW21931425) with the U.S. Environmental Protection Agency (USEPA). HELP model version 3.07, issued on November 1, 1997, is the latest version of this program and is the one used in current performance assessments. The software quality assurance plan for the use of the HELP model in Performance Assessments (PA) has been documented (Phifer 2006). It is public domain software and is available from the WES website at: http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=landfill

The HELP model is a quasi-two-dimensional water balance model that is designed to conduct landfill water balance analyses. It requires the input of weather, soil, and closure cap design data and provides estimates of runoff, evapotranspiration, lateral drainage, vertical percolation (i.e. infiltration), hydraulic head, and water storage. These estimates are used to evaluate various landfill and closure cap designs. As a water balance model, HELP has several limitations, one of which is that it does not consider transient moisture redistribution; also, this method only considers gravity as the driving mechanism for water flow (Zornberg 2007).

The National Research Council of the National Academies (NRC-NA 2007) conducted an assessment of waste barrier performance, which included information on the use of the HELP model. The NRC-NA concluded that the HELP model is probably the most widely used model to predict the water balance (infiltration in particular) of closure caps. They noted that the primary advantages of the HELP model over more sophisticated models for unsaturated flow (i.e., those solving Richard's equation and utilizing characteristic curves) are that the HELP model requires much less input data and requires significant less computational time. While the NRC-NA conceptually prefers the use of the more sophisticated models over the HELP model, their evaluation of the HELP model indicates that it over-predicts infiltration in humid environments similar to that at SRS (see NRC-NA 2007 Table 5.5). Bonaparte et al.

(2002) came to conclusions consistent with the NRC-NA 2007 regarding the use of the HELP model. Bonaparte, et al. (2002) performed a literature review of the comparison of field derived landfill water balances to HELP model results. This evaluation concluded that "for a number of cases the HELP model analysis was shown to give reasonable predictions of cumulative longer-term water balances." In addition Bonaparte et al. (2002) performed an evaluation of measured leachate collection and removal system (LCRS) flow rates for six landfill cells versus leachate generation rates estimated by HELP. Based upon this evaluation the authors concluded "that the HELP model can appropriately be employed as a tool to estimate long-term average leachate generation rates …"

3.1.2 LEACHM

LEACHM was developed by Dr. John Hutson of Flinders University. It was actively developed until 2003, with January 2003 being the latest revision to the model. It was reported that LEACHM performed adequately for run-off, evapotranspiration, and percolation (Ogorzalek 2008, Shackleford 2006).

3.1.3 UNSAT-H

UNSAT-H is a FORTRAN code used to simulate the one-dimensional flow of water, vapor, and heat in soils. It solves Richards' equation to predict the processes of precipitation, evaporation, transpiration, soil-water storage, and drainage. It is developed and managed by the Hydrology group at Pacific Northwest National Laboratory. UNSAT-H is apparently still under active use and development.

UNSAT-H was one of the codes reviewed by Benson and Shackelford and has been compared with VADOSE/W as both of these codes solve Richards equation, and both were specifically developed to evaluate the hydrology of earthen covers with vegetation (Benson 2005, Shackelford 2006). Benson et al. reported that UNSAT-H over-predicted surface runoff by an appreciable amount and was generally less accurate than VADOSE/W (Benson 2005). Ogorzalek also reported that UNSAT-H consistently over-predicted run-off, although it modeled evapotranspiration and percolation accurately (Ogorzalek 2008). The version of UNSAT-H used in these reviews was not reported.

3.1.4 SVFlux

SVFlux is an extension and adaptation of the older SoilCover model. SVFlux implements evaporative flux boundaries and is designed to be used to evaluate long-term performance of earth covers. It is currently under active development by SoilVision Systems. According to Gitirana, the performance of SVFlux is similar to VADOSE/W, with the computation of surface runoff being the driving condition for the differences in results (Gitirana 2005, Gitirana 2006). As SVFlux slightly underperforms VADOSE/W, we chose not to further evaluate this model.

3.1.5 HYDRUS-2D3D

Hydrus-2D3D is the latest version in the HYDRUS family of codes. HYDRUS 1.0 was initially developed by the US ARS and was then commercialized and further developed by the company PC-Progress into HYDRUS-2D and then into HYDRUS-2D3D. HYDRUS-2D3D is a software package that simulates water, heat, and solute movement in either two- or three-dimensional variably saturated media and is currently under active development and use.

Multiple reviews of HYDRUS-2D have been completed and comparisons with experimental work have also been carried out (Diodato 2000, Phogat 2009, McCoy 2009, Ogorzalek 2008). These comparisons have shown that Hydrus-2D is capable of accurately modeling various saturated and unsaturated flow conditions. HYDRUS-2D has been used to model transient and steady state seepage flux along with water level from soil surface as a function of time and distance from an irrigation canal (Phogat 2009). It has also been calibrated using a subset of experimental data and then validated by comparing with observed and predicted soil water contents at multiple depths over two growing conditions (McCoy 2009). Ogorzalek compares HYDRUS-2D with LEACHM and UNSAT-H, where it performs favorably: it correctly predicts total run-off, evapotranspiration (after the first year), and percolation (Ogorzalek 2008). HYDRUS-2D has been used to predict the water-flux under various vegetation coverage conditions at the Savannah River Site's E-Area Disposal Trenches (Young 2003).

The only shortcoming of these reviews is that results from the current version of HYDRUS (HYDRUS-2D3D) have not been reviewed or published in the literature. It is expected that this version should perform at least as well as the previous versions, as the only change has been expanding the code to handle 3D cases and improving the user interface.

3.1.6 VADOSE/W

VADOSE/W uses the first principles of physics as its calculator to determine the energy balance of the system. To determine this energy flow, VADOSE/W takes into account all of the flow mechanisms that can possibly occur in a system. VADOSE/W has been developed over many years and continues to be actively developed by the GEO-STUDIO company.

Benson compared the performance of VADOSE/W to other Richards' equation solving codes and they found that VADOSE/W accurately predicted surface runoff, evapotranspiration, and the temporal variations in soil water storage (Benson 2005). O'Kane et al. determined in their evaluation of various models that simulate the long-term performance of a dry cover system that VADOSE/W included more of the processes and characteristics that are important to cover system performance than other models, including HYDRUS-2D, HELP, and UNSAT-H. These processes included the formulation of the flow and transport numerical equations, the description of the boundary conditions, and the ease of using the pre- and post-processor interfaces (O'Kane 2003).

Song and Yanful compared VADOSE/W with field constructed covers and measured various geochemical and hydraulic properties. The results of this comparison showed that VADOSE/W performed very well with respect to precipitation, evaporation, , and soil water storage. It did not perform as well for predicting percolation during the winter months of the simulation due to VADOSE/W failing to treat snowfall and rain as being frozen during this time and therefore not available to percolate through the soil cover (Song 2008). Similar results were reported by Benson et al (Benson 2005). However, these results were over a small time span (3 years) and the total percolation comparison was of small order – 4 mm reported from field measurements and 0.3 mm from VADOSE/W. While the difference in magnitude may be large (factor of 13), the absolute difference (3.7 mm) is small, especially when compared with the runoff (80mm), evapotranspiration (800mm), and soil-water storage (175mm) values.

Gitirana et al. compare VADOSE/W to both experimental data and to SVFlux (Gitirana 2005, Gitirana 2006). They report that the infiltration rates using SVFlux and VADOSE/W are in close agreement, except when high precipitation rates were encountered (Gitirana 2005, Gitirana 2006). The high precipitation rates impacted the VADOSE/W performance, although it appears that poor performance only when observed at small time scales (several model days); at longer time scales (years), these problems are not noticeable (Gitirana 2005, Gitirana 2006).

The above analyses did not state which version of VADOSE/W was used. In 2007, a new version of VADOSE/W was released; this work will help determine if some of these difficulties have been addressed.

3.2 CODE EVALUATION

While many codes have been developed to model various aspects of evapotransport, runoff, and other modes of flow, only a few have incorporated all of the necessary mechanisms and algorithms to correctly determine these values. Based on the literature review, we have narrowed the choices for replacement codes to HYDRUS-2D3D and VADOSE/W. These two codes seem to be the most complete in their implementation of various environmental variables and have a well established literature and field usage background.

These two codes both solve Richards' equation for unsaturated flow, but handle plant transpiration, soil moisture curves, and other climate data in different ways. The differences in HELP, HYDRUS-2D3D, and VADOSE/W are described below.

3.2.1 Data Requirements

HELP, HYDRUS-2D3D, and VADOSE/ W are all generic computer codes that are designed to solve water-flow problems, given the appropriate user input. As a result of this, these codes require environmental data to describe the situation that is being modeled.

3.2.1.1 Climate Data

Where VADOSE/W and HYDRUS-2D3D are dependent on the user to provide all of the climatic data, HELP includes environmental data for selected US cities. HELP also provides a built-in tool to generate synthetic data for a given location, given a few basic parameters. Including this built-in data with HELP allows the user to get started with analysis right-away and provide a rough answer to a given question. VADOSE/W also includes a global climatic database; however this must be downloaded from the GEO-SLOPE website and imported into the model and has fewer locations than the HELP dataset. Neither the HYDRUS-2D3D nor the VADOSE/W codes has the capability to generate synthetic climate data.

This lack of built-in climate data does not impact PA modeling, as it incorporates known climate data, under the assumption that future climate conditions will resemble the past. VADOSE/W allows the importation of 65,536 climate data points (the limit of Microsoft Excel). The HYDRUS-2D3D graphical user interface only allows the use of approximately 15,000 climate data points. The HYDRUS-2D3D documentation claims that additional data points can be entered into one of the input files, however, this is not a straight-forward cut-and-paste operation as the fields are space delimited and require the data to be in the proper format, followed by re-importation of the climate file into the overall HYDRUS-2D3D project.

VADOSE/W accepts for its climate data: the daily maximum and minimum temperature, the daily maximum and minimum relative humidity, the daily average wind speed, the daily total precipitation, and the precipitation start and ending hour. VADOSE/W can either estimate the daily insolation, based on the location latitude, or accept as input the net radiation. It appears that these values are used to estimate the potential evaporation and transpiration, although this is not clear from the documentation. If the potential evaporation/transpiration data is available, VADOSE/W will accept it as input, and presumably use it. If the model period for VADOSE/W is longer than the provided climate data, VADOSE/W will cycle over the provided climate data.

The climate data for HYDRUS-2D3D is entered as part of the time variable boundary conditions. Unlike VADOSE/W, where climate data is limited to a daily scale, HYDRUS-2D3D accepts data at whatever time scale the model is set to (from seconds to years). The precipitation, evaporation, and transpiration are required and defined as the “model length scale” per “time scale” (e.g. m/hr). For HYDRUS-2D3D, the evaporation and transpiration values are required to be computed or measured by the user. For this analysis we used the same method as the HELP model to compute these two values (described below).

The HELP model computes the various evaporation and transpiration rates given the latitude, evaporative zone depth, maximum leaf area index, growing season start and end days, average wind speed, and relative humidity over the four quarters of the year. The equations used to compute evaporation and transpiration are found in EPA/600/R-94/168b (Schroeder 1994b) and were used to compute the evaporation and transpiration values used in HYDRUS-2D3D.

3.2.1.2 Units

Both the HELP and VADOSE/W models can accept data in either US Imperial or metric units, HYDRUS-2D3D uses only metric units.

3.2.1.3 Plant modeling

Plant modeling in VADOSE/W is done through three different inputs: Leaf Area Index (LAI), Plant Moisture Limiting (PML), and Root Depth. The LAI is a function of time, in days. This function can either be input as a spline data point function, where the LAI is plotted vs time, or the user can provide an Add-In function that describes the LAI. The PML function describes the matric suction of the plant in kPa vs a limiting factor. From the VADOSE/W help, it appears that the limiting factor is also known as the wilting point; however, this is not entirely clear from the in-program help or the VADOSE/W 2007 Engineering book. The Engineering book describes a "typical" PML as when a plant reaches a wilting point at a negative pore water pressure of about -100kPa and is completely unable to draw water if the pressure reaches -1500 kPa (Vadose 2007). The online help states that the user: "should use a function from the GeoStudio function database for all types of vegetation if you do not have any data to apply otherwise", although the location of this database was not stated, and could not be located. The Root Depth function describes how the plants' roots grow over time, where root depth is expressed in meters and the time is expressed in days.

Plant modeling in HYDRUS-2D3D was more detailed than in VADOSE/W, however, it is unclear if this extra detail improves the calculations. HYDRUS-2D3D uses a Water Uptake Reduction Model to describe root water uptake. This model either uses a Feddes or S-Shaped function, these functions are parameterized with a Critical Stress Index, which when set smaller than 1 implies root water uptake with compensation. The Feddes and S-Shaped functions are based on literature descriptions of root water uptake. These models are parameterized, the Feddes model uses seven parameters and a database of these parameters, based on different plants, is built into HYDRUS-2D3D. The S-Shaped model uses three parameters and these parameters are preset to default values, which the user can change. HYDRUS-2D3D also includes a root distribution model, which takes as input the maximum rooting depth, depth of maximum root intensity, and a parameter Pz, which is described in the HYDRUS-2D3D User manual, as an empirical parameter (Hydrus 2007). HYDRUS-2D3D also allows the user to specify the horizontal root distribution in the x-direction (2D) and y-direction (3D). HYDRUS-2D3D also contains a menu located in the Domain Properties section that defines the root water uptake values. The user selects nodes, and the menu asks for the top value (for root water uptake), and has a radio-button to toggle the type of root water uptake distribution – either the same value for all selected nodes or as a linear distribution with depth. It is unclear if this menu is altered, if it overrides the values provided by the Water Uptake Reduction Model or if it augments this function in some manner.

3.2.1.4 Soil modeling

Soil modeling in HYDRUS-2D3D requires the user to select the hydraulic model to use. In this work we use the van Genuchten-Mualem model. The user also has the option to describe hysteresis – this can be done through describing different types of retention curves. In this work we did not use hysteresis. Each type of soil is described through the van Genuchten parameters. We chose the built-in sandy-clay soil as its parameters closely match the soil found in the E-Area Trenches. If the vanGenuchten parameters are not known for the soil, adequate soil data must be provided so that these parameters can be extracted from the soil data.

Soil modeling in VADOSE/W is a little more complex than in HYDRUS-2D3D. The water content functions can be entered using their vanGenuchten parameters. The hydraulic conductivity function is entered as individual data-points, which are either determined from the vanGenuchten parameters or from measured data. The functionality to use pure vanGenuchten parameters does not function properly inside of VADOSE/W, so the data was created in Excel using the parameters and the 1980 form of the vanGenuchten equations to describe the Water Content and Relative Permeability. VADOSE/W has additional functionality to describe at what pressure PWP become activated. It is unclear from the help and users guide what PWP stands for – likely it is pore water pressure. There are additional parameters to describe the K-ratio and K-direction. These apparently impact the hydraulic function – but again, the documentation is sparse on these parameters functions.

Soil modeling in HELP is combined with the model size creation. The area of the waste-cover is defined along with the area where runoff can occur. HELP permits the input of initial soil moisture storage. If this is not specified, it is set to approximately steady-state conditions. For each soil layer, the type, thickness, and texture must be defined. There are four types of layers available to HELP – the vertical percolation, lateral drainage, barrier soil liner, and geomembrane liner. These types describe how water moves through the layer. The thickness is the thickness of the layer. The type of soil is either one of 42 built-in textures, or the user can define the type by manually filling in the reaming properties. The user must specify the drainage length, drain slope, leachate recirculation percentage, where that recirculation goes, the subsurface inflow. If the type is a geomembrane, the characteristics of that membrane must be defined as well. HELP also requires a runoff curve to be defined. The user can input their own or HELP can generate one based on slope, slope-length, soil texture of the surface layer, and the vegetation covering the surface. HELP defines the type of vegetation as ranging from bare ground to an excellent stand of grass.

3.2.1.5 Model Size and Mesh Generation

HELP sets up the model size as part of the soil definitions. Both HYDRUS-2D3D and VADOSE/W are finite element models and therefore use a grid to define each element. Each of these codes includes a mesh-generator and the user is able to specify element size. Vadose/W gives 4 mesh options: Quads and Triangles, Triangles only, Triangle Grids of Quads/Triangles, and Rectangular Grids of Quads. The HYDRUS-2D3D does not provide these types of options; it generates a mesh that prefers triangles.

3.2.1.6 Time Scale and Numerical Modeling

VADOSE/W is limited to a time scale of days or seconds in metric units, and hours in Imperial units, the HYDRUS-2D3D time scale ranges from seconds to years. The HELP model accepts daily data for precipitation, temperature, evapotranspiration, and solar radiation. Although if no daily data is provided, HELP can compute synthetic data based on yearly average measurements (Schroeder 1994)

The numerical modeling conditions are set as part of the initial model setup in VADOSE/W. The user defines the convergence criteria by the maximum number of iterations and the tolerance, which is only checked with respect to pressure head. The user can also specify the maximum and minimum changes in conductivity as well as the rate of that change. The user can also specify the type of equation solver to be used: either direct or parallel direct. In

VADOSE/W the user provides the starting time and duration as well as the number of steps and how those steps increase (linearly or exponentially). The time steps can be calculated from either Nodal Heads, Vector Norms, or from the Iteration Count. The amount of percent change in the Head per step is also a user specified parameter. Finally the user can specify the allowable time step range.

Numerical modeling in HYDRUS-2D3D is carried out over a series of time steps. The user inputs the desired time unit (ranges from seconds to years) and the initial and final times. The user specifies the initial time step, the minimum and maximum time step size. The user must also specify if the boundary conditions are time-variable or steady-state as well as the number of time-variable boundary records. As part of the numerical simulation, the user can specify the maximum number of iterations that occur at each time step as well as the final conditions that must occur for the simulation to move to the next step. These stopping tolerances are defined by the water content and the pressure head. These two tolerances had to be adjusted from the "recommended" values provided by the HYDRUS-2D3D documentation by a factor of ten. It was unclear if this was due to the simulation being carried out in nearly saturated soils in a high humidity environment or if there were other issues that needed to be addressed.

Recommendation: Similar performance for HYDRUS-2D3D and VADOSE/W.

3.2.2 Stability

Richards' equation is inherently unstable and to extract a numerical solution from it can be a challenge. In the cases examined, the sandy-clay type soil with large precipitation factors requires a change in the iteration criteria from the recommended values. The problem with this is that each iteration may not converge, introducing errors to the overall mass-balance. However, when greater tolerances are allowed, the simulation is able to complete over the given time frame.

It was also noted that when loading large data files (greater than 8MB) both VADOSE/W and HYDRUS-2D3D would occasionally quit. This usually occurred only upon loading the file and not during the actual calculation. VADOSE/W was also unstable when trying to calculate the steady-state initial conditions. It would calculate just fine for several iterations and then suddenly throw an error, asking the user to report the error to GEO-SLOPE. This type of error did not occur with HYDRUS-2D3D.

Recommendation: HYDRUS-2D3D

3.2.3 Speed

The speed of both VADOSE/W and HYDRUS- 2D3D is highly dependent upon the system being simulated and the computer upon which the model is run; however this is true of any finite element system. While neither code is as fast as HELP, the type of calculations being computed precludes this being the case. HYDRUS-2D3D is reasonably fast, with the average run time taking less than 10 minutes to calculate 15,000 hours of time-step data.

VADOSE/W took approximately 6 hours to calculate the same type of time-step data, although the iteration criteria in both codes were similar.

Recommendation: HYDRUS-2D3D

3.2.4 Accuracy

We need to ensure that the new Richards' equation based models are indeed more accurate and not simply more precise than the water-balance method. Although the codes that solve Richards' equation are more sophisticated than the water-balance models, they are challenging to use to predict small percolation values over long lengths of time with a high level of accuracy. This is due to multiple reasons, one of which is that the mass balance errors produced by the numerical models tend to be of the same order of magnitude as the percolation values. (Zornberg 2007).

The accuracy of the candidate codes is better described in section 3.3, where we evaluate each code in comparison to a demonstration problem.

Recommendation: Both HYDRUS-2D3D and VADOSE/W should be carefully checked for this type of error.

3.3 EVALUATION OF TEST PROBLEMS

We thought to do a head to head comparison of HYDRUS-2D3D and VADOSE/W by using identical inputs and comparing the output to determine the difference in the codes. This was more of a challenge than initially anticipated, for several reasons: the large amount of climate data that had to be gathered and manually validated, computed, and formatted; the different codes use different mechanisms to describe root distribution and root water uptake, these differences had to be discerned and accounted for; the different codes use different atmospheric boundary conditions, how these are implemented had to be discovered.

3.3.1 Simple simulation

Before modeling a complex site, like the F-Tank Farm cover cap, we thought to test the different codes on a simple simulation. This simple simulation was of a section of ground that is 15m wide at the bottom by 10.3m (left side) and 10m (right side) deep. The differences in the depth are caused by the top having a 2% slope from right to left (See Figure 1. Simple Simulation). The sides were marked as no flow boundaries, the bottom was defined as having a constant pressure head of 0m, and the top boundary was defined as the climate (VADOSE/W) or atmospheric (HYDRUS-2D3D) boundary condition. The mesh was defined to be 1m elements in the top half of the modeled zone and 2m elements in the bottom half of the modeled zone.

We obtained climate data obtained from the SRS Weather Center for the years 1994-2009. This data included precipitation, relative humidity, wind speed, and solar radiation. The time frame of this simulation was five years, we used data from 1996-2001.

For the soil properties, we used the van Genuchten parameters that were built into HYDRUS-2D3D for 'Sandy-Clay' soil. Initially, the model would not run to completion (of the 5 years) using the ‘Sandy-Clay’ parameters and the recommended numerical modeling parameters. By tweaking these parameters to allow larger tolerances between iterations (changing from the default Water Content Tolerance from 0.001 to 0.01 and Pressure Head Tolerance from 0.05 to 0.1), we were able to complete the simulations using HYDRUS-2D3D. Using these looser tolerances, we obtained a percolation value of 17.6 in/yr.

We ran into a similar problem of non-completion with VADOSE/W. In that code, after approximately 8 days (model time) the code began to take infinitesimally small time steps. After tweaking the tolerances the code ran to completion and we were able to obtain some results.

A HELP code simulation for this scenario produced an infiltration estimate of 9.8 in/yr using USDA Sandy Clay and a fair grass cover.

3.4 RELATIVE COSTS AND BENEFITS

3.4.1 Marginal costs

There are distinct costs involved with switching modeling platforms and part of this report is to determine those costs.

One of the primary factors associated with switching to a model based on Richards’ equation is that those codes require a more detailed set of climate data than the HELP code. However, to complete this report we have obtained that set of data, and have transformed it into a form that either HYDRUS-2D3D or VADOSE/W can use; therefore, that is not as large of an issue as it could be.

Other costs involved with switching codes include issues with the soil properties, numerical simulation (the inherent instability of Richards’ equation), mesh generation, and result extraction.

Most of the time/effort put into these models is involved with getting the data in the proper format and determining the soil properties and boundary conditions that will generate stable numerical simulations.

Also, the time to learn a new system, as well as to be able to test and correct for any modeling deficiencies (numerical instability) is not insignificant.

3.4.2 Marginal benefits

HYDRUS-2D3D offers the potential for improved predictive accuracy by using a Richards’ equation based model versus a water-balance model. However, our limited testing was insufficient to definitively conclude that HYDRUS-2D3D simulations will be more accurate than HELP.

4.0 CONCLUSIONS

1) The 1996-2009 Central Shops data from the SRS Weather Center, assembled and formatted in this study, are recommended for climate input in future SRS cover system analyses involving transient solution of Richards' equations (HYDRUS-2D3D, VADOSE/W, etc.).

2) HYDRUS-2D3D and VADOSE/W were judged to be the best current alternatives to HELP based on a survey of the open literature. The largest difference between the two codes is their approach to modeling evaporative transpiration. VADOSE/W uses a first principles approach while HYDRUS-2D3D uses empirical equations. HYDRUS-2D3D does not account for snow fall or melt-runoff. So, while snow is not a large factor at SRS, that may be a major concern at other sites across the DOE complex (Hanford, Idaho, etc).

3) Based on a subsequent hands-on evaluation, HYDRUS-2D3D is the preferred over VADOSE/W for the following reasons:

> a) The HYDRUS family of codes is <u>more widely known and used</u>. Earlier versions of HYDRUS are available to the public free of cost. These may be important considerations to reviewers and other stakeholders.
>
> b) The <u>licensing cost is much lower</u> for HYDRUS-2D3D. Twenty perpetual network licenses for HYDRUS were purchased for approximately the same cost at one perpetual hardware key locked VADOSE/W license.
>
> c) As indicated by the name, HYDRUS-2D3D <u>includes a 3D capability</u>. While 2D is sufficient for most cover systems, analysis of discrete holes in HDPE and GCL liners may require 3D simulations.
>
> d) HYDRUS-2D3D is <u>capable of simulating general multiphase flow and transport</u>, whereas VADOSE/W simulates liquid flow.
>
> e) The <u>Graphical User Interface (GUI) was more robust</u> for HYDRUS-2D3D during our limited testing. The VADOSE/W GUI regularly exhibited a fatal error that prevented completion of numerical simulations. We did not pursue a bug fix with the developers.

4) For a simple no-cover scenario (Sandy Clay soil type and grass cover), HYDRUS-2D3D produced an infiltration estimate of 17.6 in/yr. For a similar problem specification (USDA SC soil and fair stand of grass), the HELP model produces an estimate of 9.8 in/yr. Both model predictions are within the range of infiltration estimates generated from field measurements and other modeling studies for similar conditions (cf. WSRC-STI-2007-00184, Rev. 2, Table 9).

5) The merits of using HYDRUS-2D3D over HELP for cover system scenarios are still uncertain at this point. Evaluation of additional scenarios and parameter settings would be needed to assess any systemic biases in HYDRUS-2D3D relative to HELP and/or field measurements for SRS applications.

6) Since none of the currently available codes is perfect and as part of the long-term planning process, it may be worthwhile to consider investing in one of the open-source codes (UNSAT-H or others) and modifying that code to provide the needed functionality. The advantages of this would be: the code would be available – many people could look at it's source and find errors that might otherwise go undetected; the code could be modified as needed to add functionality and take advantage of new techniques in numerical modeling; and be continuously improved upon.

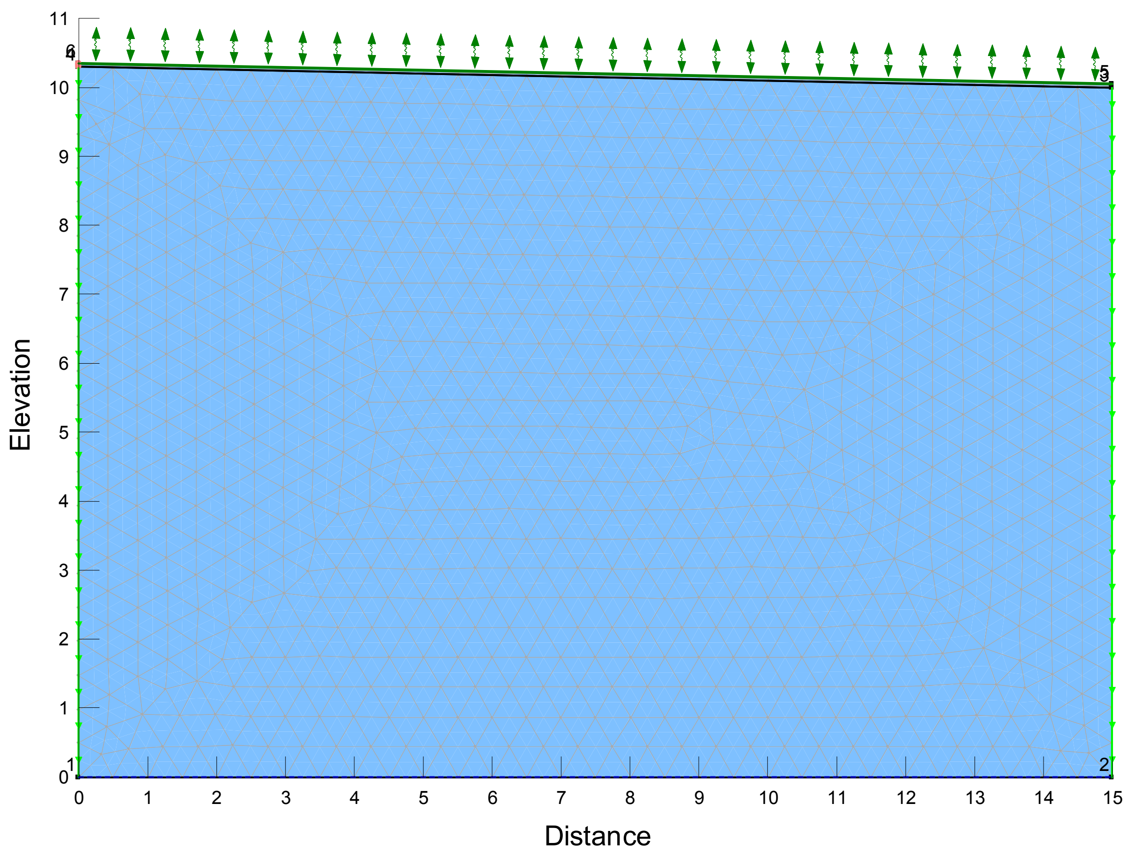

Figure 1. Simple Simulation

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