Numerical Modeling in Geoenvironmental Practice

By Craig H. Benson, Ph.D., P.E., M.ASCE

Modeling of non-linear systems is now a regular part of geoenvironmental engineering practice due to the availability of inexpensive, high-speed PCs that utilize user-friendly software and graphical user interfaces. Robust and efficient solvers for non-linear partial differential equations have also had a major impact on the practicality of geoenvironmental software packages. Consequently, detailed analyses are being done in practice that were not possible a decade ago. These include realistic assessments of potential performance as well as "what if" scenarios. The most common analyses are associated with vadose-zone hydrology to predict the movement of water in the vadose zone and interactions with the atmosphere. However, contaminant transport analyses in variably saturated systems are also becoming commonplace.

Software Resources

A variety of powerful codes are available. The most common codes used for analysis of vadose zone hydrology and unsaturated flow are HYDRUS (www.pc-progress.com), UNSAT-H (www.hydrology.pnl.gov or www.uwgeosoft.org), VADOSE/W (www.geoslope.com), SEEP/W (www.geoslope.com), and SVFLUX (www.soilvision.com). HYDRUS is the most commonly used code in vadose zone hydrology worldwide, and can also be used to simulate heat flow and contaminant transport in unsaturated media. Other software packages commonly used for contaminant transport simulation in variably saturated media include CTRAN/W (www.geoslope.com), CHEMFLUX (www.soilvision.com), and STOMP (www.stomp.pnl.gov). Three-dimensional simulations are possible with HYDRUS, SEEPW, SVFLUX, CHEMFLUX, and STOMP. Versions of HYDRUS are also available that simulate variably saturated reactive transport using equilibrium and kinetic geochemical algorithms (www.sckcen.be/hp1/).

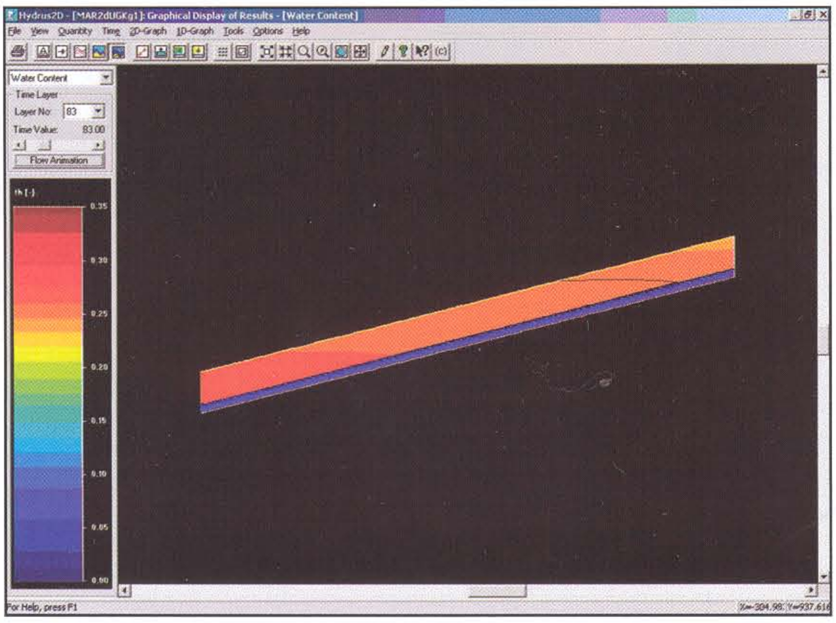

Figure 1. Example of distribution of volumetric water content in a sloping section of a water balance cover employing a capillary barrier located in Monterey, CA. Predictions were made with HYDRUS-2D. Low water contents exist in the coarse-grained layer near the base that forms the capillary break. Higher water contents exist in the fine-textured layer used for water storage. The variation in color in the fine-texture layer (orange-red color) shows the down-slope diversion of water due to the capillary break.

Applications

Typical output from a HYRDUS-2D simulation is shown in Figure 1. This simulation considered a sloping landfill cover with a capillary break (fine layer over coarse layer). The image shows the contrast in water content at the capillary break (orange colors for higher water contents in the upper finer-grained layer; blue colors for low water contents in the coarse-grained underlying layer). Accumulation of water down slope in the finer-grained upper layer is also evident. The accumulation is caused by lateral diversion in the finer-grained layer that is induced by the capillary break between the layers. Another example of output from HYDRUS-2D is shown in Figure 2. The image shows sulfate

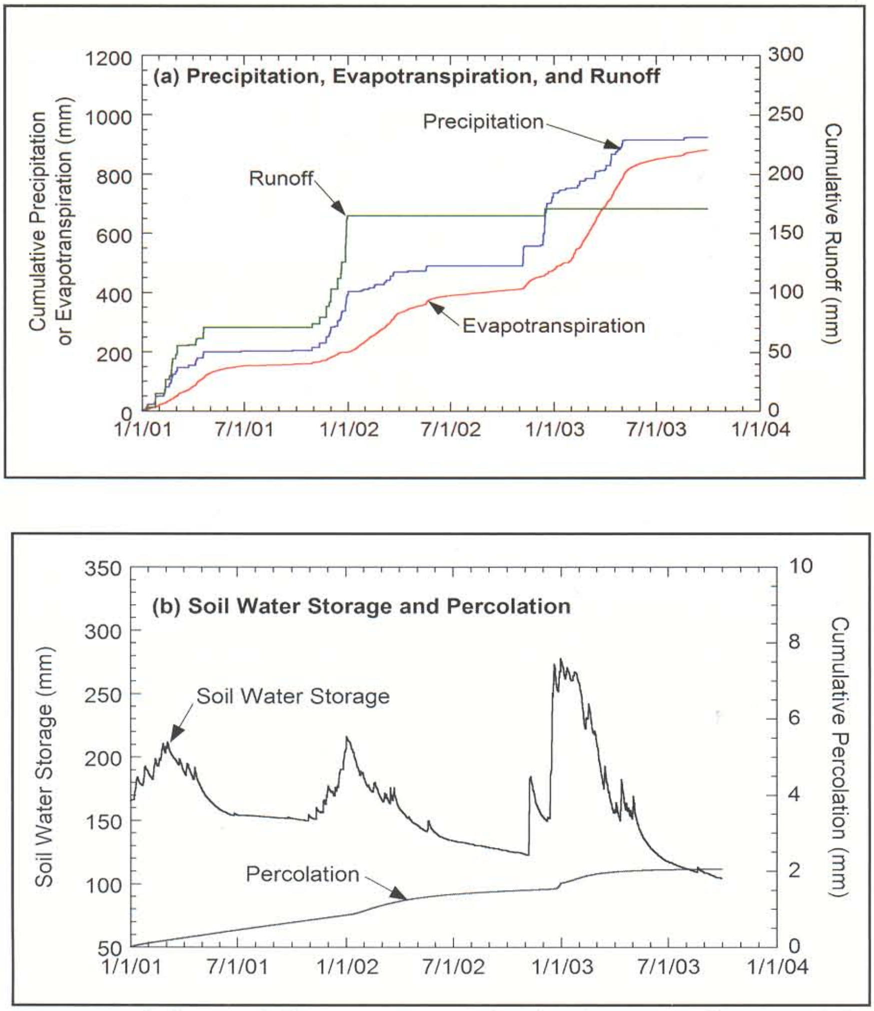

Figure 3a and 3b. Water balance quantities predicted with UNSAT-H for a monolithic final cover over a solid-waste landfill at a semi-arid location: (a) precipitation, evapotranspiration, and runoff; (b) soil water storage and percolation. Soil water storage is the total volume of water in the cover per unit area. The variation in soil water storage reflects the seasonal variation in degree of saturation within the cover profile.

"realistic." Understanding the accuracy and limitations of numerical models is critical, particularly sophisticated models of highly non-linear systems that have many options. Most certainly, model predictions must always be tempered with engineering judgment and checked by others with modeling expertise.

Parameterization

Parameterization remains a major factor affecting the accuracy of predictions made when modeling geoenvironmental systems. Scale effects and bias can have a significant impact on the primary variables that are commonly measured (e.g., saturated hydraulic conductivity, the soil water characteristic curve, partition coefficients). However, other less conspicuous variables can also have an important effect on the accuracy of predictions. For example, the unsaturated hydraulic conductivity function is rarely determined experimentally because of the difficulties associated with its measurement. Instead, an inference is normally made using a capillary-tube model and parameters describing the soil water characteristic curve. The most common model is the van Genuchten-Mualem function, an analytical expression relating unsaturated hydraulic conductivity to suction or volumetric water content. An important variable in this function is the pore interaction term, which generally is assumed to be 0.5. Recent studies have shown, however, that this term can range from 0.5 to 3.0, which can have a dramatic effect on the rate at which the unsaturated hydraulic conductivity decreases as the suction increases.

The predictions in Figure 4, made with UNSAT-H, show that cumulative evapotranspiration varies by as much as 30% depending on the magnitude of the pore interaction parameter used in the simulation. A variation this large could have a significant effect on the viability of the cover design. This example illustrates that expertise in parameterization can be as important as expertise in numerical methods when making predictions in geoenvironmental engineering using numerical models.

Training

Predictions made with numerical models depend on a variety of factors, including the parameters used as input, the boundary conditions selected, and the spatial and temporal discretization employed. Understanding how these factors affect predictions is essential. For example, an engineer recently called to ask: "what is this van Genuchten α parameter in the unsaturated hydraulic properties input?" Clearly, this engineer did not have the training necessary to be conducting numerical modeling of unsaturated flow problems. Numerical modeling requires more than a person to "turn the crank" and collate the output. Even if the software can easily be run by point-and-click input, the modeler needs training to ensure that the model is set up properly, the input is realistic, and the predictions are accurate and reasonable.

Conclusion

The numerical models available to today's geoenvironmental engineer are extremely powerful. They can be used to solve problems that could not be analyzed in practice a decade ago. Many of the models also have sophisticated interfaces that make input and operation simple and efficient, and the output can appear extremely realistic. However, engineers must not forget that models are always an

concentrations in a tailings disposal facility. The analysis considered variably saturated flow due to drainage of the tailings, water and oxygen ingress from an overlying cap, and geochemical reactions within the tailings due to the oxygen source in the cap.

Non-linear numerical models are essential for analyzing scenarios such as those shown in Figures 1 and 2. They cannot be analyzed directly with analytical solutions. Many of the software packages used to conduct non-linear modeling have been developed commercially and must be licensed. However, some are available in the public domain. For example, HYDRUS-1D is an extremely powerful public-domain software package that can handle non-linear flow and transport problems in one dimension. The software can simulate a variety of sophisticated problems, including colloidal transport (using filtration theory), atmospheric interactions including snow melt and root water uptake, heat transport, CO_2 transport, and carbonate chemistry. Forward simulations can be conducted for prediction, and inverse simulations can be performed for parameter estimation from field and/or laboratory data.

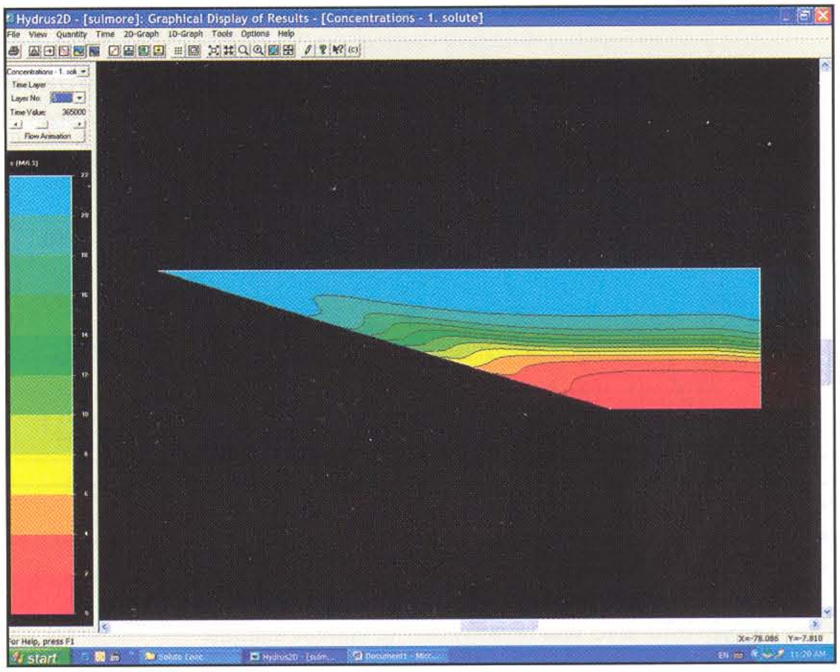

Figure 2. Sulfate concentrations (g/L) in a tailings disposal facility during drainage of the tailings. HYDRUS-2D was used to simulate unsaturated flow and contaminant transport within the tailings facility. (Courtesy of Hong Kim, HKK Consultants, Reno, NV.)

Model Predictions Versus Reality

One of the most common geoengineering applications of software for vadose zone hydrology is for the design of water balance covers used for landfill closures. Water balance covers function by storing infiltration in unsaturated fine-textured soil with minimal percolation into the underlying waste, and then releasing the stored water to the atmosphere via evaporation and transpiration. Numerical modeling is conducted to verify that the cover will function as intended using actual metrological data as input. What-if simulations are also conducted to evaluate scenarios such as loss of vegetation by fire, unusual precipitation events, or the impacts of pedogenesis (i.e., changes in soil structure and engineering properties in response to physical, chemical and biological weathering).

The most commonly used software packages for analyzing water balance covers are UNSAT-H, HYDRUS, and VADOSE/W. SVFLUX is also becoming more commonplace. All of these codes solve Richards' partial differential equation for unsaturated flow and include a sink term for root water uptake. Richards' equation is highly non-linear because the unsaturated hydraulic conductivity varies orders of magnitude as the suction (or saturation) varies. An example of a water balance prediction made with UNSAT-H is shown in Figure 3a and 3b. In this case, a 900-mm-thick water balance cover was simulated for a three-year period for a landfill at a semi-arid site in California. The design required that the percolation rate through the cover not exceed 3 mm/yr. As shown in Figure 3b, the design criterion is met, at least for the three year period simulated.

The output shown in Figures 3a and 3b appear remarkably realistic. The runoff and soil water storage curves appear jagged which reflect the rapid response of these water balance variables to episodic precipitation events. In contrast, the evapotranspiration and percolation curves are smoother, reflecting how damping and averaging within the profile affect these fluxes. But danger lies in the realism. The output can appear so realistic as to be taken as truth, whereas the accuracy of the predictions greatly depends on the algorithms used in the software and the reliability of the input parameters. In addition, the software can be so complicated that errors go unnoticed even with extensive benchmark testing. For example, in a recent study, disparate results were obtained with two widely used and well-documented software packages. Investigation into the discrepancy showed that one software package contained an error that was affecting the predictions. Differences in algorithms can also have an important effect on the output. For example, in a recent study, a comparison was made between predictions from four different software packages used for simulating water balance covers. Identical input was used in each case. The comparison showed that the software packages provide similar trends in the water balance quantities, but the numerical values predicted by each package were different.

The take-away message is that models are an approximation of reality. Thus, predictions made with a numerical model are *not reality*—even if the predictions appear very

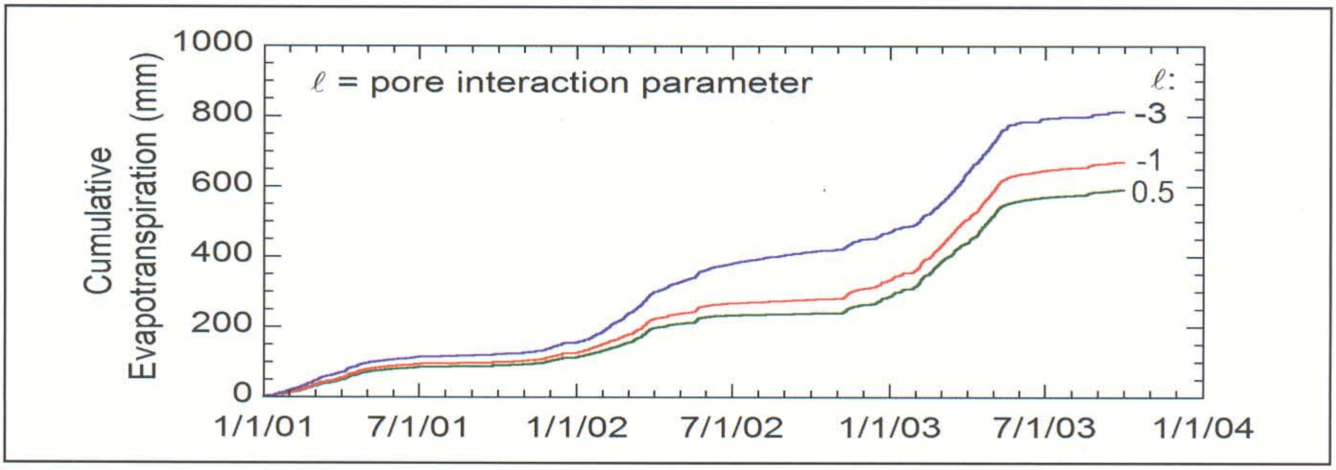

Figure 4. Predictions of cumulative evapotranspiration from a monolithic water balance landfill cover made with three values of the pore interaction parameter. In most cases, the pore interaction parameter is implicitly assumed to be 0.5.

abstraction of reality, and that predictions must always be considered in the context of field data and experience. The importance of parameterization and user training cannot be underestimated, as the predictions made with any numerical model are only as reliable as the data used as input and the expertise of the engineer conducting the modeling. ❍

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