Model Complexity and Model Validity: Application to the Las Cruces Trench Experiment, INTRAVAL Test Case 10

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ABSTRACT

Safety assessments of geologic high-level radioactive waste repositories require the use of predictive models to describe specific processes which may affect the fate and transport of radionuclides and determine the performance of each of the subsystems, as well as that of the overall repository system. However, many uncertainties exist in the procedure of developing a conceptual model which incorporates the relevant physico-chemical processes, mathematically formulating this conceptual model, and numerically implementing the mathematical model. Whether or not the impact of these uncertainties is such that the chosen model may be considered sufficiently accurate for performing safety assessments is a fundamental issue which has motivated studies of model validation as applied to high-level waste (HLW) repository analysis. The international INTRAVAL project has as its aim the development of concepts for improving and validating mathematical models which describe the flow and transport of radionuclides in the geosphere.

To develop and test validation concepts, the INTRAVAL project has assembled seventeen test cases which have produced data from either laboratory or field experiments or from natural analog studies which are suitable for quantitatively assessing the accuracy of flow and transport models. The Las Cruces Trench Site in southeastern New Mexico is one of four INTRAVAL test cases conducted in hydrologically unsaturated porous media. The Las Cruces Trench experiment is situated in unconsolidated alluvium, while the experiments at the Apache Leap Site, G-Tunnel, and Yucca Mountain involve unsaturated fractured rock. Although these last three test cases are more directly relevant to the U.S. HLW repository program at the proposed Yucca Mountain site, the extensive characterization of the soil hydraulic properties and detailed monitoring of the infiltration experiments makes the trench ideal for analyzing issues related to model validity and site characterization.

To assess the effects of model complexity on the accuracy of model predictions, a series of conceptual (and corresponding numerical) flow models were constructed for the Plot 2b experiment at the trench. The least complex model consisted of nine horizontal zones, roughly corresponding to the nine identified soil horizons, within which the soil hydraulic properties were assumed to be constant. For the nine layer conceptual models the soil hydraulic properties were determined by simultaneously fitting the van Genuchten model to the water retention curves obtained from all soil samples taken within a given soil layer. The more complex conceptual models consisted of 121 and 3621 rectangular zones, whose soil hydraulic properties were assigned by kriging the van Genuchten model parameters and saturated hydraulic conductivity estimates obtained from each of the soil samples.

Quantitative comparison of predicted water contents to measured water contents obtained from neutron probes were made using two different performance measures. Based on the sum of squared differences between measured and predicted water contents over space and time, the most complex model produced the most accurate predictions. However, comparative analysis of the first and second moments of the water content distribution as functions of time leads to equivocal results. Analysis of the second moments of the water content distribution indicates that there is less variation among the three conceptual models than between the models and the experimental results. This last observation suggests that there is a consistent source of bias in the model predictions; an observation confirmed by visual inspection of the computed and measured wetting fronts. All three conceptual models fail to predict the horizontal bifurcation of the observed water content plume which occurs at a depth of approximately 2.5 m. This apparent bifurcation is believed to be due to the presence of a relatively coarse, sandy soil layer capable of transmitting high water fluxes in the unsaturated regime without a measurable increase in water content. The existence of this sandy layer is confirmed through spatial analysis of the soil particle size distribution. Soil samples taken in this horizon to obtain water retention data apparently failed to capture the hydraulically distinct behavior of the sand. If the bifurcation of the plume was hypothesized to be crucial to some regulatory decision, then one would have to draw the conclusion that all of the conceptual models considered here have failed the validation criteria. However, it is not clear that the bifurcation of the plume would indeed lead to a different regulatory decision in this hypothetical example.

These results suggest that efforts should be made to define *a priori* those features that may affect the flow field to the extent of impacting a regulatory decision. These definitions should then be periodically updated as more site data becomes available. Thus, site characterization will be an iterative process in which the data interpretation through modeling and definition of data needs are coupled and site characterization and model validation proceed in parallel. While full validation of site-specific conceptual models is not possible, confidence sufficient for appropriate regulatory decision can be gained by designing this coupling appropriately.

INTRODUCTION

Investigation of model validity requires that a conceptual (and corresponding mathematical) model has been formulated, that a set of data is available by which its validity may be judged, and that rules for judging model validity have been defined. Any conclusions reached as to the validity of the model critically depend on the choices made for these three attributes.

The level of simplification at which the basic conservation equations are written, the adoption of particular constitutive relationships, the scale at which the heterogeneity of the experimental domain is represented, the level of discretization for numerical purposes, and the solution method are all part of formulating the model. Inasmuch as many choices are possible during model formulation, it is rarely the case that a single model can be called uniquely correct. For example, it is possible to formulate models of varying complexity using one set of site characterization data simply by altering the methods used to map measured initial conditions and material properties to the model. Obviously, additional site characterization data may lead to formulation of additional models within the set of applicable models.

Generally, the data used for model formulation and the data used for validation are required to be independent of each other. In the case discussed here, the validation data set was indeed independent, and in fact was not made available to the modelers until after their model predictions were completed. The validation data set exhibited features whose presence would not have been predicted from the portion of the site characterization data used to construct the model. To be specific, the soil hydraulic property data alone were not sufficient to account for a site feature whose presence turned out to greatly affect the movement of the moisture plume. It needs to be stated that the data came from a carefully designed and executed model validation experiment and therefore it can not be assumed that the crucial site feature was missed due to oversight. How much additional field data was needed to select a correct model, although difficult to determine, is critical to deciding the appropriate level of site characterization.

Whether the lack of agreement between the movement of the predicted moisture plume and that of the measured plume demands that the model be categorically rejected depends upon the criteria used for judging model validity. If accurate prediction of the shape of the plume was the sole criterion, then obviously the model is rejected. However, if the criteria include performance measures other than plume shape (e.g., the mass of water crossing a specified compliance boundary), then the model may not be rejected. From the above discussion, it is apparent that models for performance assessment of a HLW repository probably cannot be validated in any absolute sense, but only with respect to appropriate site characterization and appropriate validation criteria. The greatest benefit that such tests of numerical models against precisely defined experiments have is to buoy the analyst's and regulator's faith that the numerical model, when correctly applied, captures the underlying physics.

This work is a result of the authors' participation in the international INTRAVAL project on the validation of geosphere transport models for performance assessment of nuclear waste disposal. The particular validation data set used here is known as test case 10, the Las Cruces trench experiment which is conducted in unconsolidated alluvium. The extensive characterization of the soil hydraulic properties and detailed monitoring of water contents and solute concentrations at the Las Cruces trench make it well suited for developing and testing model validation strategies.[1] Phase 1 of INTRAVAL focused on validating models of both unsaturated flow and solute transport for the Plot 2a experiment for which the measured water contents and solute concentrations for both bromide and tritium were released to the modelers prior to model predictions. In Phase 2, INTRAVAL study participants used the model developed in Phase 1 to predict the outcome of the experiment prior to the release of the experimental data. Results of Phase 2 will be discussed here. All models developed to date for this study of the Plot 2b experiment, as well as those of the Plot 2a experiment, have used the PORFLOW, Version 1.2 (single-phase version) computer code to simulate the flow of water and transport of tracers.

EXPERIMENTAL SETTING

The experimental trench is located northeast of Las Cruces, New Mexico, on the New Mexico State University College Ranch near the north end of the Doña Ana Mountains. The climate at the experiment site is semi-arid. Class A pan evaporation is 239 cm per year, while average annual precipitation is only 23 cm, over half of which falls during the summer monsoon season. As shown in Figure 1, the trench is 26.4 m long, 4.8 m wide, and 6 m deep. Plot 2, located adjacent to the north face of the trench, is irrigated by an array of 80 drip lines aligned parallel to the trench face and covering a surface strip 12 m long and 1.2 m wide. During the Plot 2b experiment, water was applied to the strip at a rate of 1.82 cm/day for 70 days. Chromium, boron, and pentafluorobenzoic acid were applied to the strip during the first 15 days, and tritium, bromide, and 2,6-difluorobenzoic acid were applied during days 29 through 44.[1] Water content was monitored by neutron probes through the network of access tubes shown in Figure 1. Matric potential was monitored by tensiometers installed

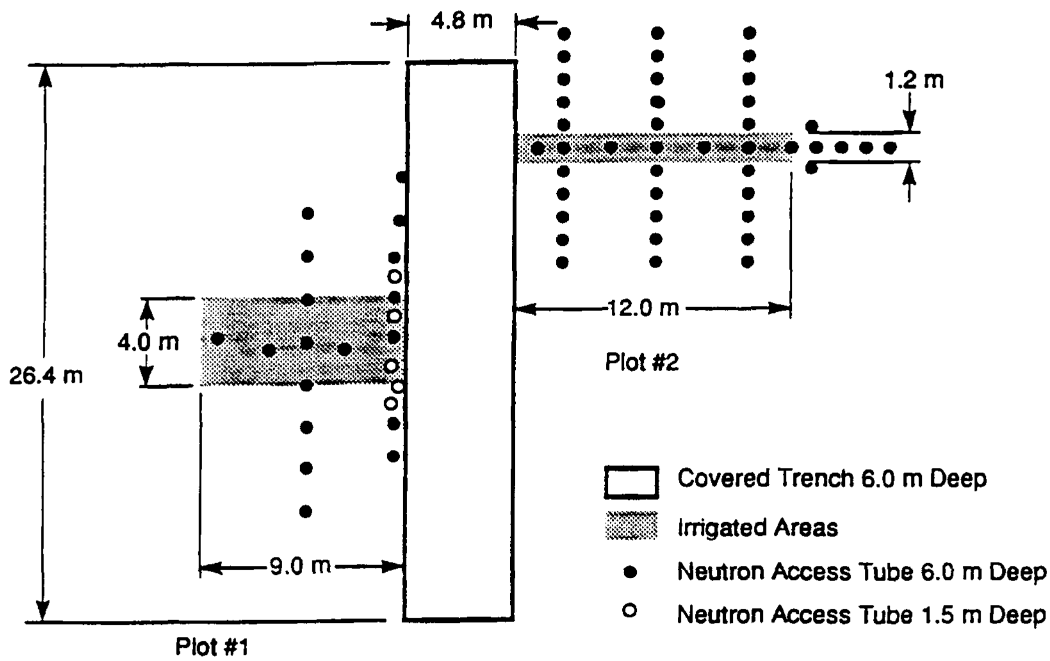


Figure 1. Plan view of the Las Cruces trench.

in the face of the trench. Solute samples were obtained using suction lysimeters installed in the trench face and destructive sampling of small diameter soil cores at selected locations to the north of the trench.

DETERMINATION OF SOIL HYDRAULIC PROPERTIES

Approximately 600 soil cores and 600 disturbed soil samples were taken during the construction of the trench. Fifty samples of each type, spaced at 50 cm intervals, were taken along nine horizontal transects corresponding to the nine soil layers identified in the north face of the trench.[1] In addition, samples were taken along three vertical transects at a spacing of 13 cm. Water retention data were obtained from the soil cores by determining water content at suctions of 10, 20, 40, 80, 120, 200, and 300 cm H_2O. The high suction end for each of the water retention curves was determined from crushed and sieved portions of the disturbed soil samples which were placed in pressure plate extractors and subjected to pressures of 1, 5, and 15 bar.

The van Genuchten model [2] was used to describe the water retention or moisture characteristic curve. This model is given by

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{[1 + (\alpha h)^n]^m} \tag{1}$$

where θ_r is the residual water content, θ_s is the saturated water content, h is suction head, and α, m, and n are unknown fitting parameters. It is further assumed that $m = 1\text{-}1/n$, which facilitates the derivation of a closed-form expression for the unsaturated hydraulic conductivity as a function of water content or pressure head based on Mualem's predictive model for the unsaturated hydraulic conductivity.[3] The van Genuchten-Mualem model for unsaturated hydraulic conductivity is

$$K(h) = K_s \frac{\{1 - (\alpha h)^{n-1}[1 + (\alpha h)^n]^{-m}\}^2}{[1 + (\alpha h)^n]^{m/2}} \tag{2}$$

where K_s is the saturated hydraulic conductivity.

During previous modeling of the Plot 2a experiment considerable difficulty was encountered in determining a suitable set of initial pressures, since many of the water content values measured by neutron probes were less than the residual water contents.[1] It was assumed that the soil hydraulic parameters, which were determined from cores taken in a vertical cross-section parallel and immediately adjacent to the north face of the trench, could be directly projected normal to the north trench face and made coincident with the planar arrays of neutron probe access tubes at 2, 6, and 10 m from the face. Any node, i, in the computational mesh that resides in the intersection of the rectangular areas of influence for soil sample location, l, and the neutron probe location, j, was assigned the pressure head

$$h_i = \frac{1}{\alpha_l}\left[\left(\frac{\theta_j - \theta_{r_l}}{\theta_{s_l} - \theta_{r_l}}\right)^{\frac{n_l}{1-n_l}} - 1\right]^{n_l} \tag{3}$$

Although Eq. 3 is defined when $\theta_j < \theta_{rl}$, this condition implies negative saturation, and the pressure head predicted by Eq. 3 is meaningless. To resolve this problem the pressure head at any node for which this condition occurred was set to 15 bar, the pressure at which the residual water contents was defined.[1] Consequently, the estimated initial water content in many portions of the model domain exceeded the measured water content.

To eliminate this difficulty for the Plot 2b study θ_r, α, and n were re-estimated for each of the water retention curves. An estimation procedure suggested by Mualem whereby θ_r, α, and n are determined subject to the constraint that the computed water retention curve passes through the point corresponding to the highest suction and lowest water content was implemented using constrained nonlinear least squares.[3] Approximately 100 soil samples for whose retention curves the minimum water content did not coincide with the highest applied suction were removed from consideration. Unfortunately there remained some locations in the model domain where the re-estimated residual water content still exceeded the measured initial water content. This problem was finally resolved by including an additional point to each set of water retention data consisting of the lowest water content measured by neutron probe and the highest suction measured by thermocouple psychrometer, followed by re-estimation of θ_r, α, and n.

PARAMETER ZONATION AND MODEL CONSTRUCTION

The van Genuchten model parameters re-estimated from the water retention data and the saturated hydraulic conductivities determined *in situ* using Guelph permeameters were mapped to specified zones of the computational mesh using two distinct procedures. The first procedure was used to construct the parameter zonation for the least complex model used in this study, which consisted of nine parameter zones corresponding to the nine distinct soil layers observed on the north side of the trench face. Using the first procedure, the van Genuchten parameters for each zone were determined using the constrained estimation procedure described above for all water retention data from that horizontal transect. The second procedure used kriging to determine the parameter values for the more complex models used in this study. The more complex models consisted of 121 and 3621 rectangular parameter zones defined on regular grids of 11×11 and 51×71, respectively, in the horizontal and vertical directions.

In previous work on the Plot 2a experiment, a simple rectangular area of influence procedure was employed to directly map the soil hydraulic properties to the finite difference mesh used in PORFLOW. This resulted in the model's parameter zonation having a distinctly "blocky" structure which may have unduly amplified the lack of spatial continuity in the parameters. In addition, because this area of influence method is a zeroth order interpolation procedure, it fails to either filter out or smooth the noise in the parameter data. To improve the spatial smoothness of the hydraulic parameter data, punctual kriging was used to map the soil hydraulic data to the parameter zones for both the 121 and 3621 zone models.

The spatial structure of the field saturated hydraulic conductivities from the Las Cruces Trench has been analyzed in detail.[4] This analysis indicates that an anisotropic exponential semi-variogram with horizontal and vertical correlation lengths of 2.5 and 0.5 m, respectively, a nugget of 0.4, and a sill of 1.54 adequately fits the sample semi-variogram constructed for the logarithm of hydraulic conductivity. The exponential model with nugget is given by

$$\gamma(x) = \begin{cases} 0 & x = 0 \\ C_0 + C_1\left[1 - \exp\left(\frac{x}{l}\right)\right] & x > 0 \end{cases} \qquad (4)$$

where C_0 is the nugget, C_1 is the sill, and l is the correlation length. This semi-variogram was used to krige the saturated hydraulic conductivity. For the other soil hydraulic parameters, the correlation lengths and range determined for the *in situ* K_s were assumed; however, the sill for each parameter was set equal to its variance. For all parameters, kriging was performed in a local neighborhood with a radius of 2.5 m, with 5 nearest neighbors allowed per quadrant.

The computational mesh used for the 9-zone, 121-zone, and 3621-zone models, as shown in Figure 2, consists of 81 nodes in the horizontal and 97 nodes in the vertical direction. The mesh is increasingly refined towards the center and top of the domain to accommodate the large pressure head gradients expected to occur at early time directly below the strip source. Boundary conditions were everywhere defined to be no-flow, except at the bottom of the model and at the 1.2 m horizontal

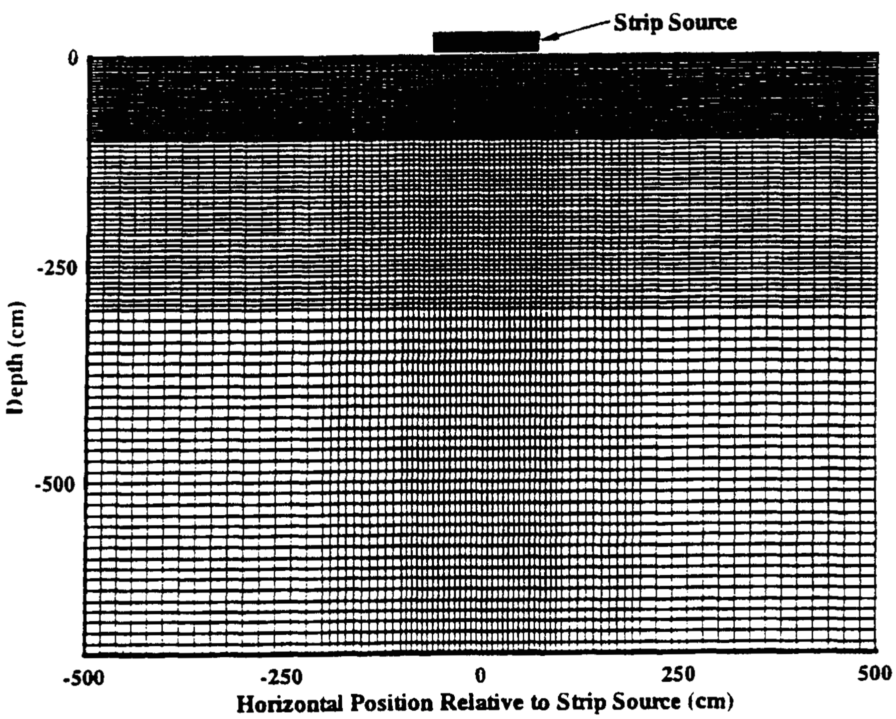


Figure 2. Computational mesh.

portion at the top where the strip source is located. To simulate gravity drainage, a negative pressure head gradient of unit magnitude was specified at the bottom of the domain. At the strip source, the boundary condition was prescribed flow type set equal to 1.82 cm/day during the first 70 days of simulation and zero thereafter.

MODEL RESULTS AND COMPARATIVE MEASURES

Simulations for each of the three models were performed for each of the three transects located at 2, 6, and 10 m (transects 1, 2, and 3, respectively) with model results recorded for 55 different time periods over the 310-day simulation time. Each PORFLOW model run took approximately 100 central processing unit (CPU) minutes on the CRAY Y-MP8/4-64 at Los Alamos National Laboratory (LANL) and generated a 70 Mb plot file. Because of the large quantity of data both generated by the models and obtained from the actual experiment, very few contour plots of either the computed or measured water content are included here.

Computer animation studies indicate that, while the model results do appear to replicate the overall rate of translation and spread of the wetting front, there are fundamental features of the observed flow regime that none of the models capture. In particular, animated sequences of the contoured measured water content data reveal a vertical bifurcation of the moisture plume at all transects at approximately 3 m depth. Thus, it appears that, at 3 m depth, there exists a distinct horizontal layer of soil whose hydraulic properties permit transmission of water at much lower water contents than do the rest of the layers. Figures 3a through 3d are contour plots of water content along transect 1 at day 75 for the experimental data, the 9-zone model, the 121-zone model, and the 3621-zone model, respectively. For Figures 3a through 3d the darker shades indicate higher water contents while the lighter shades indicate lower water contents. Figure 3a shows the pronounced split in the water content plume, a feature clearly not evident in Figures 3b through 3d. Visual inspection also reveals that there is greater similarity among the three model results than between any of the models and the measured water contents. This observation is the first suggestion that there is a consistent source of bias in the model predictions.

PLUME MOMENT ANALYSIS

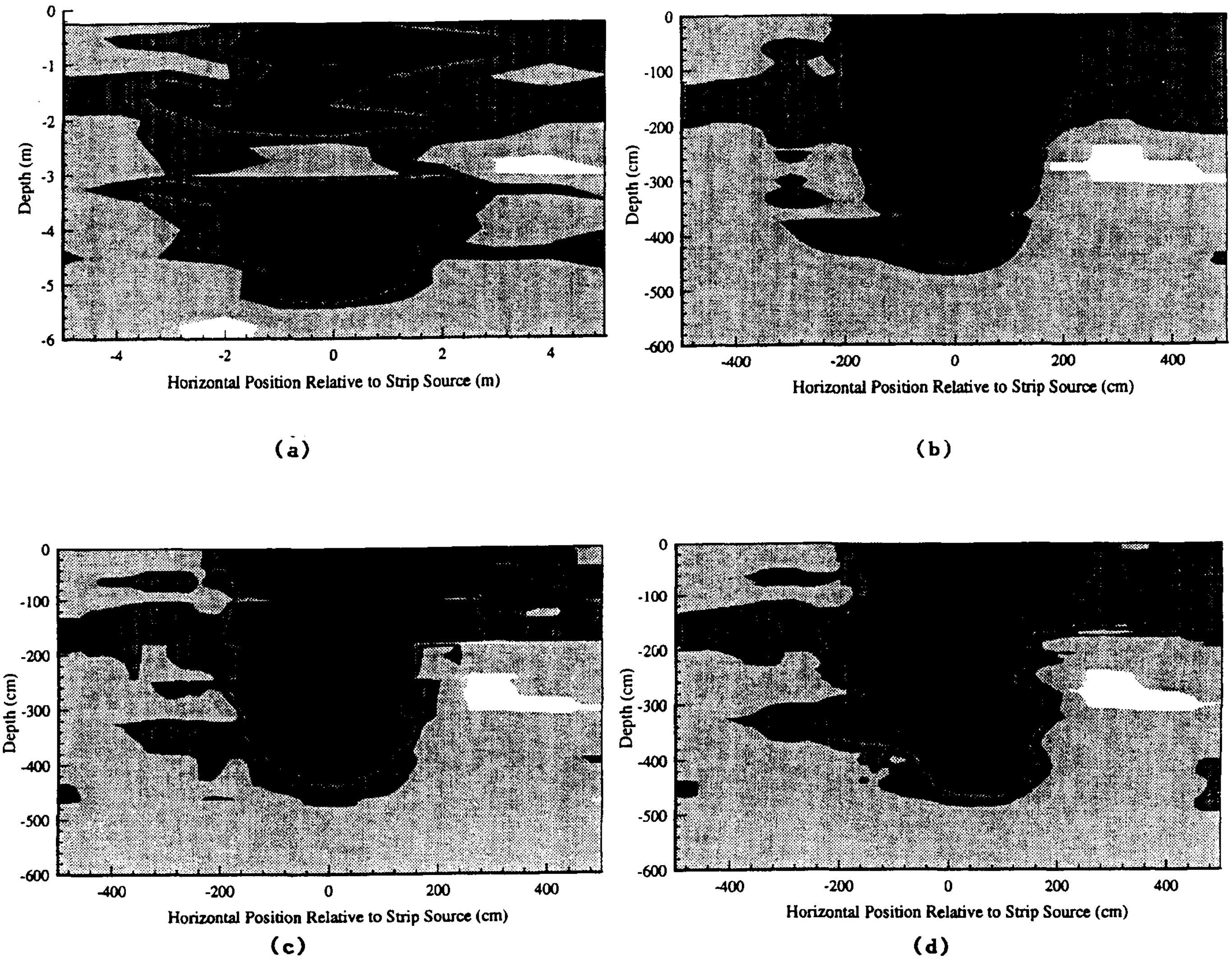
To quantitatively compare the rate of translation and spread of the computed and measured wetting fronts, the first and second moments of the difference in water contents between time 0 and the time period of interest were computed. The moment of order, l, in the x-direction, and k in the z-direction is

$$M_{lk} = \iint_{zx} [\theta(x,z,t_0) - \theta(x,z,t)] x^l z^k dx dz \tag{5}$$

where $\theta(x, z, t_0)$ and $\theta(x, z, t)$ are the moisture contents at point (x,z) and times 0 and t, respectively. The x and z coordinates of the plume centroid are

$$X_c = M_{10} / M_{00} \tag{6}$$

$$Z_c = M_{01} / M_{00} \tag{7}$$



Figures 3a-3d. Contours of water content at day 75: (a) measured; (b) predicted, 9-zone model; (c) predicted, 121-zone model; and (d) predicted, 3621-zone model.

The centroid is used to represent the mean position of the plume, while the second moment about the centroid is used to represent the extent of the spread of the plume about its center. Equations for the three second moments are

$$S_{xx} = M_{20} \ / \ M_{00} - X_c^2 \qquad (8)$$

$$S_{zz} = M_{02} \;/\; M_{00} - Z_c^2 \tag{9}$$

$$S_{xz} = M_{11} \;/\; M_{00} - X_c Z_c \tag{10}$$

The square roots of the second moments have units of length and are interpreted as measures of plume spread. The mixed second moment reflects the degree of asymmetry of the plume.

The x and z locations of the centroid of the water content difference plumes at transect 1 for all sample times are shown for the measured data, the 9-zone model, the 121-zone model, and the 3621-zone model in Figures 4a and 4b. At early times, there is considerable variability in the x-coordinate of the centroid of the measured water content difference plume. This variability may reflect errors introduced when data were interpolated to those neutron probe locations at which samples were not taken every time. The variability is also due in part to the error propagation effect that results from taking differences between initial water contents and those measured at later times.

The horizontal position of the measured plume shows a slight 10 cm deviation to the right of the center of the strip source after 150 days. As expected, the 9-zone model shows little deviation about the horizontal; however, the 121-zone model predicts that the center of the plume should drift some 25 cm to the right of center. In contrast, the 3621-zone model predicts that the moisture plume should move to the left of center some 10 cm after 310 days. As can be seen in Figure 4b, all of the models roughly approximate the rate of vertical movement of the plume centroid, although the 3621-zone model most closely approximates that of the measured data. Again, there appears to be less variability among the model predictions of the centroid of the water content difference plume than between those predicted and that measured.

In computing the second moments about the mean for the measured data, the same numerical difficulties and consequent variability in moment estimates described above can be seen in Figures 4c and 4d, although the effects are less pronounced. All of the models slightly overpredict the vertical spread of the water content difference plume at later times and underpredict the horizontal spread at later times. The 3621-zone model more accurately predicts the overall dispersion of the plume than do either of the less complex models.

POINT-TO-POINT COMPARISONS

Comparisons of point predictions of water content to measured water content at transect 1 made with the use of scatter plots neither support nor refute the conclusions reached on the basis of comparing moments that the 3621-zone model is more accurate. If the model predictions were accurate it would be expected that the scatter plot points would all fall on the 45-degree line that passes through the origin. The extent to which these points lie scattered about the 45-degree line provides some qualitative sense of the validity of the model. Simple statistical tests of significance on the regression coefficients for a straight line fit to these points have been used to quantitatively judge the validity of models.[5] This analysis has not been performed on these data, however, the scatter plots indicate that all three models on average tend to over predict the water contents.

Calculating the sum of squared differences between measured and predicted yields a directly comparable measure of scatter. Figure 5 is a plot of the cumulative sum of squared differences

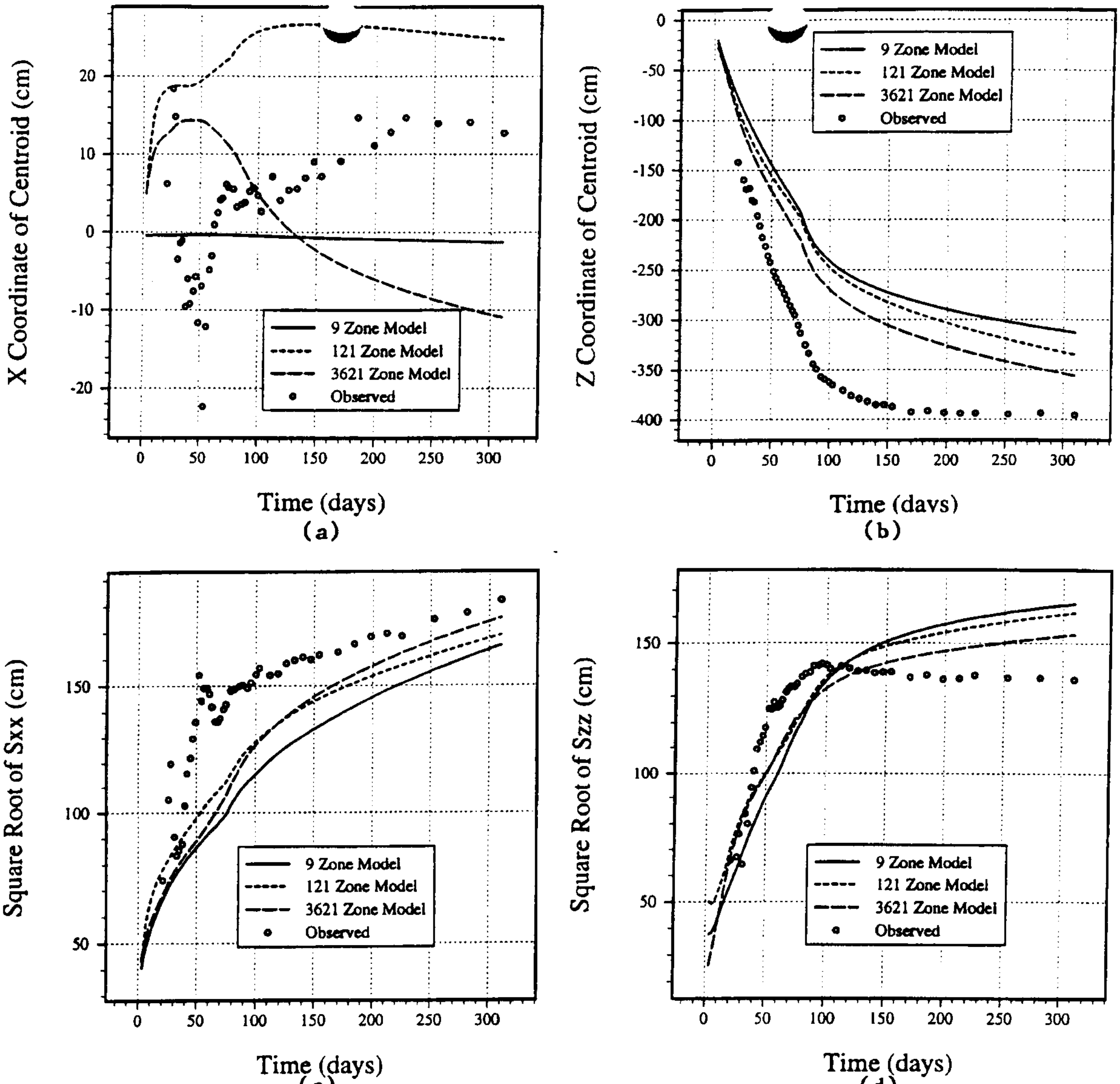


Figure 4a-4d. Moments of water content difference plumes: (a) X-coordinate of centroid; (b) Z-coordinate of centroid; (c) square root of second moment about the centroid in the X-direction; and (d) square root of second moment about the centroid in the Z-direction.

between measured and computed water content at transect 1 as a function of time. Because the actual measurement locations were included as a subset of the computational nodes used in the models, and because of the care taken in converting the measured water contents to pressure heads, the cumulative sum of squared residuals at day 0 is zero for all three models. Once sufficient water has infiltrated to change the antecedent moisture conditions, the cumulative sum of squared residuals increases rapidly, with the rate of increase diminishing rapidly during the redistribution phase. The 3621 zone model produces the smallest cumulative sum of squared differences over the entire simulation period. This

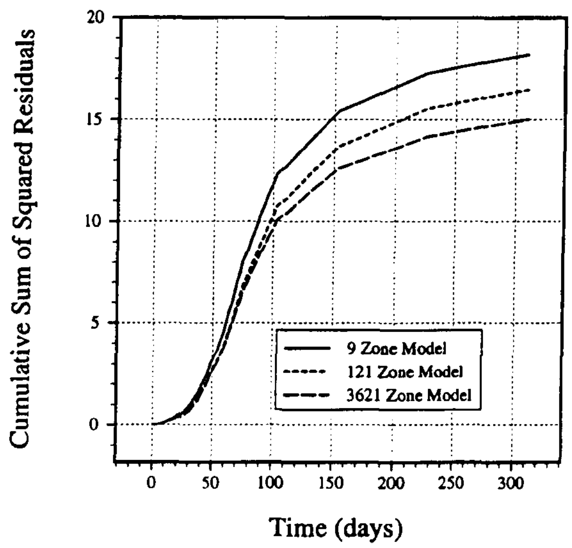


Figure 5. Cumulative sum of squared differences between measured and predicted water contents.

result supports the conclusion based on the analysis of moments that the 3621 zone model is the most accurate.

CONCLUSIONS ON MODEL COMPLEXITY AND VALIDITY

Based on the relatively simple quantitative comparative measures used to assess model validity, it appears that, at least for transect 1, the 3621 zone model most accurately predicts the actual movement of the moisture plume. However, the apparent three orders of magnitude increase in model complexity from the 9-zone model to the 3621-zone model probably greatly overstates the actual increase in complexity and should not be used to make inferences regarding the need for exhaustive site characterization. It is essential that one keep in mind that the amount of characterization data used to construct each of these models was identical and the increase in model complexity was achieved solely by altering the quantitative procedures used to interpret and map the data to the model.

It has been proposed[6] that the complexity of a model be quantitatively summarized by its degrees of freedom

$$N_F = D_E N_E N_B \tag{11}$$

where N_E is the effective number of cells with different material types, D_E is the effective spatial dimension of the flow domain, and N_B is the number of flow regions originating from boundary sources. Based on this, the degrees of freedom for the 9-zone, 121-zone, and 3621-zone model are 18, 242, and 7242, respectively. However, this measure fails to account for the degree of spatial correlation in the material heterogeneity. To account for spatial correlation, it has been proposed[6] that N_E be replaced by

$$N_E^* = \prod_{i=1,\ldots,D} \left(\frac{L_i}{\lambda_i}\right) \tag{12}$$

where L_i is the domain size along each axis, and λ_i is the correlation scale along that axis. By this definition, the effective degrees of freedom for both the 121-zone model and the 3621-zone model is 112. However, unlike Eq. (11), this measure fails to capture the increased spatial smoothness of the 3621-zone model's material properties over those of the 121-zone model.

There are other factors which appear to eliminate some of the differences in complexity among the models and thereby explain the similarity of their results. In particular, the initial pressure head conditions for each model, which are based on the same 11 × 24 array of measured initial water contents, induce a great degree of similarity in the predicted water contents at early times for those models that have fewer material zones than initial condition zones. This suggests that Eq. (11) be replaced by

$$N_F^* = D_E N_E^* N_B N_I \tag{13}$$

where N_I is the effective number of cells with different initial pressure head conditions. Thus, the degrees of freedom, N_F^*, for the 9-zone, 121-zone, and 3621-zone models are 4752, 29568, and 405552, respectively.

The similarity of the model predictions may be attributed to factors other than the above noted fact that the apparent increase in model complexity probably overstates the actual dissimilarity among the models. Based on the analysis of the moments of the water content difference plumes, there appears to be less variability among the models than between the models and the observations. This suggests that the models are plagued by a common conceptual model error. Indeed, inspection of animated sequences of the contoured water content data for both the models and the measurements reveals that all models fail to predict the vertical bifurcation of the plume which occurs at a depth of approximately 3 m. Subsequent spatial analyses of the grain size distribution data for the soil cores indicated the presence of a thin, but distinct, coarse sandy layer at an approximate depth of 3 m. Those soil samples taken within the soil horizon containing the thin sandy layer for determination of the soil hydraulic properties clearly failed to capture the capability of the sand unit to transmit relatively large water fluxes without a measurable increase in water content.

It is obvious that the set of applicable conceptual and mathematical models would need to be updated as site characterization proceeds. Regardless of the criterion selected, model validation is intimately tied to site characterization and the two must be conducted in an iterative manner. Models should be used to identify those unidentified features at the site which may affect flow and transport to an extent that regulatory decisions will be altered. Efforts should then be made to discover such features at the site and, if found, these should be included in the model and their direct regulatory impact assessed.

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