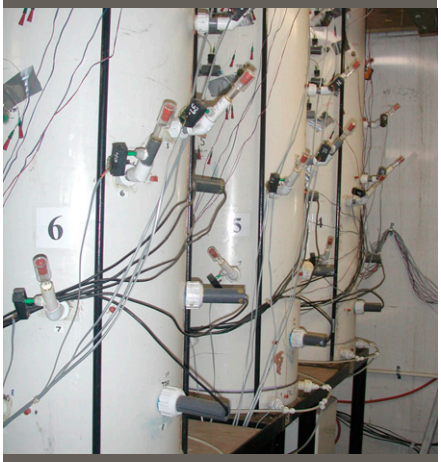
Original Research

T.H. Skaggs*
D.L. Suarez
S. Goldberg



Advanced numerical simulation models can potentially improve irrigation and soil salinity management, but prediction uncertainties need to be quantified. In this study, prediction intervals generated by propagating soil parameter uncertainties tended to underestimate the range of tracer transport variability observed across large lysimeters.

U.S. Salinity Laboratory, 450 W. Big Springs Rd., Riverside, CA 92507. *Corresponding author (todd.skaggs@ars.usda.gov).

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Effects of Soil Hydraulic and Transport Parameter Uncertainty on Predictions of Solute Transport in Large Lysimeters

Advanced numerical simulation models can potentially help improve guidelines for irrigation and salinity management. Many simulation model parameters have considerable uncertainty, and ideally that uncertainty should be reflected in model predictions and recommendations. In this work, we investigate solute transport predication intervals that can be generated by propagating model parameter uncertainty using Monte Carlo techniques. Flow and transport is simulated with a standard numerical model, while soil parameters and their uncertainty are estimated with pedotransfer functions. Generalized global sensitivity coefficients are computed to determine the parameters having the greatest impact on transport prediction and uncertainty. Simulations are compared with Br transport measured under unsaturated conditions in large lysimeters packed with clayey soil materials. In a 48 cm tall, homogeneous soil profile, model prediction intervals provided a reasonably good description of a single, relatively "noisy" breakthrough curve. In replicated 180 cm tall, layered soil profiles, model structural errors limited the accuracy of the prediction intervals under one irrigation water treatment, whereas under another treatment the predictions tracked the time course of the data reasonably well but tended to overestimate solute concentrations. The width of the prediction intervals tended to be small relative to the range of transport variability that existed across replicated lysimeters, particularly at shallow depths. Additional work aimed at operational field testing of model prediction uncertainty is needed if advanced water management models are to reach their full potential.

Abbreviations: HRU, hydrologic response units.

Although tremendous capabilities exist for modeling vadose zone hydrological processes (Šimůnek and Bradford, 2008), specifying the uncertainty in model predictions remains a significant problem. Part of the difficulty in accounting for uncertainty lies in the fact that there are many different kinds of models, with many different purposes, and no single best approach to uncertainty exists (Beven, 2009). Rather, specific models and model applications—each having characteristic model structures, data, and informational constraints—need to be investigated and best practices need to be determined. Complete model testing requires both (i) scientific evaluation in which a model's general agreement with current scientific understanding is tested; and (ii) "functional" or "operational" evaluation in which model prediction accuracy is evaluated quantitatively in the context of a particular model application (Willmott et al., 1985; Klemeš, 1986; Loague and Green, 1991; Vereecken et al., 1992; Wösten et al., 2001).

Our focus is modeling solute transport in the context of salinity management in irrigated agricultural systems. Maintaining agricultural productivity in irrigated lands requires that salts introduced by irrigation be periodically leached from soils. Several recent studies (Letey and Feng, 2007; Corwin et al., 2007; Dudley et al., 2008; Ben-Gal et al., 2008; Letey et al., 2011; Oster et al., 2012; Suarez, 2012) have suggested that classical guidelines for salinity management (U.S. Salinity Laboratory Staff, 1954; Rhoades, 1974; Ayers and Westcot, 1985) overestimate the leaching requirement as well as the negative impacts of irrigating with moderately saline waters. Accordingly, the traditional guidelines possibly encourage over-irrigation, which wastes water and increases contaminant transport to groundwater.

The traditional recommendations are based on a steady state analysis of irrigated soils, and it has been proposed that transient-state analyses, performed with well-known advanced numerical simulation models, could lead to more effective water and salinity management (Corwin et al., 2007; Letey et al., 2011; Oster et al., 2012; Suarez, 2012). A re-assessment of

guidelines for irrigation and salinity management is timely given that water availability for irrigated agriculture in arid and semiarid regions is decreasing, forcing a greater reliance on recycled or otherwise degraded waters, and a greater use of marginal quality lands.

The degree to which transient-state modeling can improve water management depends on the accuracy of the model simulations. As a practical matter, routine recommendations must be made using the models in a purely predictive mode because it will not be possible to run, for example, a solute transport experiment that would permit the calibration of model parameters. In such a scenario, model parameter values will be uncertain, and ideally that uncertainty should be reflected in the model prediction and recommendation.

Oster et al. (2012) evaluated several well-known models suitable for transient-state analyses. All of the surveyed models used the Richards equation to model variably saturated water flow and an advection-dispersion equation to model solute transport. Important model parameters include soil hydraulic parameters such as the hydraulic conductivity and transport parameters such as the dispersivity. In cropped scenarios, root water uptake and crop stress tolerance parameters are also essential.

Our objective was to examine the effects of soil hydraulic and transport parameter uncertainty on predictions of solute transport, and to consider whether such uncertainty could be used beneficially in predictions of salt accumulation and leaching. We do not address this issue, or the larger question of salinity management with transient state models, in a general or comprehensive way, but instead focus more narrowly on predictions of solute transport and uncertainty for a particular soil system, comparing predictions with transport data measured in large lysimeters over distances that are comparable to the root zones of agronomic crops. Thus this work constitutes a necessary step in what must be an incremental accumulation of basic knowledge about uncertainties in models of irrigated agricultural systems, and about methods for treating uncertainty.

Specifically, in this work we explore solute transport prediction intervals that may be generated by propagating model parameter uncertainty using the Monte Carlo method. Flow and transport is simulated with the HYDRUS-1D model (Šimůnek et al., 2005). Hydraulic parameters and their uncertainty are estimated with the Rosetta pedotransfer function (PTF) model (Schaap et al., 2001). Generalized global sensitivity analyses are presented to determine the parameters having the greatest impact on transport prediction and uncertainty.

Background

A vast literature exists on stochastic methods for subsurface hydrology, as summarized in books by Dagan (1989), Gelhar (1993), and Zhang (2002), among others. The impetus for much work on stochastic methods has been subsurface heterogeneity. Many early efforts modeled hydraulic conductivity and other material properties as spatial random fields, with transport equations developed for the mean and variance of the solute concentration (or pressure head). An alternative approach developed specifically for the vadose zone is stochastic stream tube modeling, wherein flow and transport in a field is conceived to occur in independent, one-dimensional soil columns (e.g., Bresler and Dagan, 1979; Jury and Roth, 1990). A local-scale transport model is specified for the columns, and field-average transport is determined based on the assumed random variation of local-scale model parameters across the field.

Despite the abundant research, it is generally acknowledged that stochastic theories and approaches have rarely been adopted for the management of real-world problems (Dagan, 2002; Zhang and Zhang, 2004; Renard, 2007). Among other impediments, the use of stochastic methods in vadose zone hydrology is hindered by the fact that assumptions invoked in some stochastic models such as stationary random material properties are typically not applicable to field soils (Jury and Roth, 1990). Also, it is very difficult to obtain reliable statistical information about soil spatial variability (e.g., Russo and Jury, 1987).

Moreover, heterogeneity is only one of many sources of uncertainty affecting model applications. More generally, uncertainty enters the modeling process through informational constraints regarding boundary conditions, model structures, model parameters, etc. (Beven, 2009). For example, distributed parameter modeling approaches divide the landscape into areas that are treated as independent homogeneous units, sometimes called hydrologic response units (HRUs). The delineation of HRUs might, for example, coincide with map units from a soil survey. Although the distributed approach is often viewed as a deterministic modeling framework, in practice uncertainty enters into model calculations from many sources. At the HRU scale, uncertainty exists in specifying a suitable local model, and once specified, in specifying appropriate model parameter values. When models developed from consideration of lab- or plot-scale processes are used as the HRU process model, difficulties associated with model incommensurability arise (Beven, 2009), including the impossibility of directly measuring model parameters. Parameters must therefore be estimated, and their values are necessarily uncertain (Brown and Heuvelink, 2005). A standard approach to uncertainty analysis is to specify uncertain model parameters in terms of probability density functions, and to propagate the uncertainty through the model using Monte Carlo methods or other techniques (Brown and Heuvelink, 2005).

In this context, one well known approach for estimating unknown soil parameters and their uncertainty is pedotransfer functions (e.g., Pachepsky and Rawls, 2004; Vereecken et al., 2010). Because most pedotransfer functions (PTF) have been developed from soil properties that were measured or analyzed at lab or plot scales (Jana et al., 2007), their parameter estimates can be considered incommensurate with field scale calculations. Nevertheless,

several researchers have considered the effects of PTF-estimated parameter uncertainty on model predictions. As noted by Brown and Heuvelink (2005), making progress toward "policy-relevant" modeling in hydrology and environmental sciences will likely require some balance between physical and statistical reality on one hand and pragmatism on the other. Some recent examples of PTF-uncertainty propagation include: Stenemo and Jarvis (2007), who evaluated the effects of PTFs on pesticide leaching by sampling PTF regression errors and propagating them through a simulation model in a Monte Carlo analysis; van den Berg et al. (2012), who similarly used Monte Carlo uncertainty propagation in evaluating pesticide leaching to groundwater; and Loosvelt et al. (2011), who evaluated the impact of PTF-derived soil hydraulic parameter uncertainty on soil moisture modeling. A shortcoming of these and other similar studies is that the generated prediction uncertainties were not evaluated against measured data. Although in the present work we consider only plot scale processes and data, we do so with an eye toward the development of modeling practices associated with field-scale management problems.

Methods and Materials

Transport Experiment

Skaggs et al. (2012) recently reported results for a soil salinization and leaching experiment conducted in 12 cylindrical lysimeters measuring 46 cm in diameter and 197 cm tall (Fig. 1). The lysimeters were packed with homogenized soil materials to create 12 identical soil columns having a three-layer soil texture profile: a 0- to 100-cm clay loam surface layer, a 100- to 130-cm silty clay middle layer, and a 130- to 180-cm sandy loam bottom layer. Figure 1 gives the percentages of sand, silt, and clay for each material, plus the packed bulk density for the layers. The soil materials were excavated from agricultural lands in western San Joaquin Valley, CA, and were ground and sieved before being packed in 10-cm depth increments. The three-layer soil texture profile was patterned after a west San Joaquin Valley cotton and tomato field mapped by Shouse et al. (2006). The bottom of each lysimeter had a vacuum drainage system consisting of a 10 cm sand layer which enveloped ceramic candles that were connected to a constant vacuum source (35 kPa). Instrumentation included tensiometers and solution samplers installed at eight depths. The lysimeters were installed in a rhizotron facility such that their top edges extended 18 cm above surface grade. The lysimeters were kept shaded from direct sunlight.

A 13th lysimeter, called the evaporimeter, was installed on an electronic balance and used to monitor evaporation under the nonstandard evaporation conditions that existed for the lysimeter installation. The evaporimeter had the same diameter as the other lysimeters but was only 65 cm tall (Fig. 1). The evaporimeter was packed with 48 cm of the clay loam material used in the surface-layer of the other lysimeters, had the same vacuum drainage system as the other lysimeters, and was installed in the rhizotron so that the surface conditions were the same. Regular, automated

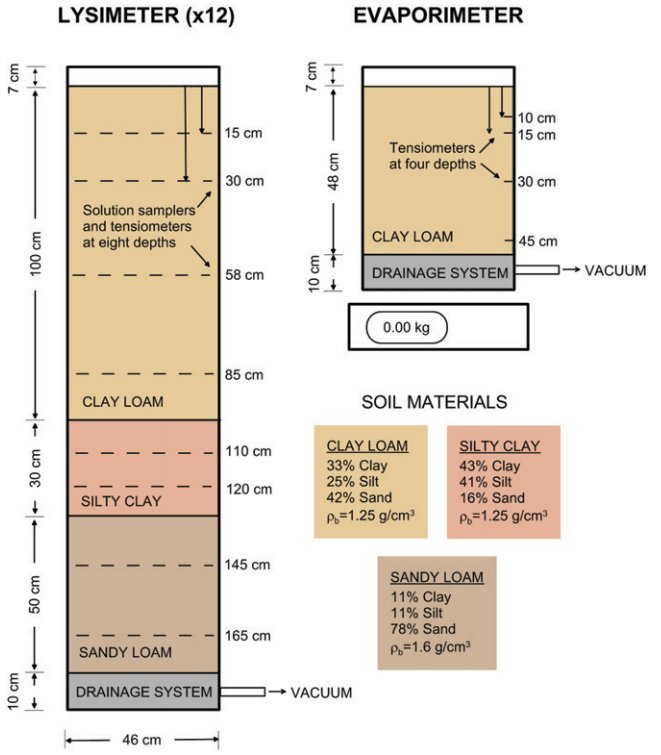

Fig. 1. Schematic illustration of the lysimeter system used in the transport experiments of Skaggs et al. (2012).

measurements of changes in the lysimeter and drainage water masses were used to determine daily values for evaporation. Full details of the construction and installation of the lysimeters and evaporimeter are given in Skaggs et al. (2012).

The experiment reported by Skaggs et al. (2012) had two irrigation phases. During the first phase, which lasted 804 d, six lysimeters were regularly irrigated with low salinity (EC = 0.4 dS m^{-1}) synthetic waters containing 20 ppm Br, while six were irrigated with high salinity (8.3 dS m^{-1}) synthetic waters also containing 20 ppm Br. During the second phase, which lasted 895 d, all lysimeters were regularly irrigated with low EC waters (0.4 dS m^{-1}) that contained only trace amounts of Br. Throughout, all lysimeters were irrigated at the same time and received the same amounts of irrigation water. Thus, with respect to Br transport, the experiment comprised six replications of two experimental treatments: treatment 1, in which Br was applied in a low EC irrigation water followed by leaching with a low EC water; and treatment 2, in which Br was applied in a high EC irrigation water followed by leaching with a low EC water. At all times, the same amount of Br and water was applied to all 12 lysimeters.

Figure 2 shows the record of lysimeter irrigations. Irrigation typically occurred three times per week. The amount applied per irrigation varied, with the goal being to obtain as high a water application rate as possible while still maintaining unsaturated soil

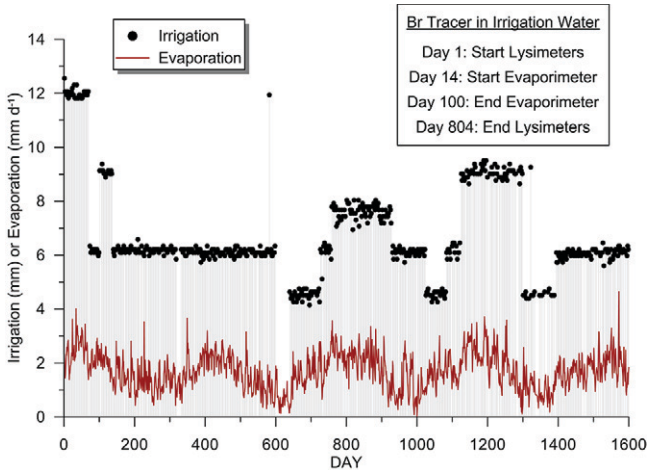

Fig. 2. Record of lysimeter (and evaporimeter) irrigations, and the evaporation rate measured with the evaporimeter. The text panel indicates the periods in which Br tracer was added to the irrigation waters. (Redrawn from Skaggs et al., 2012).

conditions (as indicated by tensiometer readings). Because of the low permeability of the soil materials, particularly the middle silty clay layer, the rate that could be maintained turned out to be quite low, with the net water application, averaged over the duration of the experiment, being less than 1 mm d^{-1}.

Figure 2 also shows the evaporation rate determined with the evaporimeter. Near the beginning of the experiment, a pulse of Br was added to the evaporimeter irrigation water for a short period (Fig. 2). Over the course of the experiment, the Br concentration in the soil solution of the lysimeters was monitored using the solution samplers installed at eight depths, and in the drainage waters of the lysimeters and evaporimeter. See Skaggs et al. (2012) for full details.

Modeling

Simulation model

Simulations of water flow and solute transport were performed using the HYDRUS-1D model. Šimůnek et al. (2005) provide a full description of the complete code; we present here a summary of the components used in our calculations.

One-dimensional variably saturated water flow in soil was modeled with the Richards equation,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z} + K(h)\right] \qquad [1]$$

where θ [L^3 L^{-3}] is the volumetric water content, h [L] is the pressure head, K [L T^{-1}] is the hydraulic conductivity, t [T] is time, and z [L] is the vertical space coordinate. The soil hydraulic properties were modeled using the van Genuchten–Mualem constitutive relationships,

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \left(1 + |\alpha h|^n\right)^{-m} & h < 0 \\ 1 & h \geq 0 \end{cases} \qquad [2]$$

$$K(h) = K^* S_e^L \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \qquad [3]$$

where $m = 1 - 1/n$, θ_s [L^3 L^{-3}] is the saturated water content, θ_r [L^3 L^{-3}] is the residual water content, K^* [L T^{-1}] is a matching point hydraulic conductivity for $S_e = 1$, and n, α [L^{-1}], and L are adjustable parameters. Although K^* is usually equated with the saturated hydraulic conductivity, $K^* = K_s$, a fitted matching point conductivity for slightly unsaturated conditions, $K^* = K_0 < K_s$, may be preferable for modeling unsaturated soils since saturated flow is typically dominated by macroporosity that does not affect unsaturated flow (Schaap and Leij, 2000; Weynants et al., 2009). Schaap and Leij (2000) observed that optimal fitted values of K_0 were often about an order-of-magnitude smaller than K_s.

Solute transport was modeled using the advection-dispersion model,

$$\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial C}{\partial z}\right) - \frac{\partial qC}{\partial z} \qquad [4]$$

where C is the solute concentration [M L^{-3}], q is the volumetric water flux density [L^3 L^{-2} T^{-1}], and D is the dispersion coefficient [L^2 T^{-1}]. The dispersion coefficient was specified as $D = \lambda q/\theta$, where λ [L] is the dispersivity.

HYDRUS-1D uses a Galerkin finite-element method to solve the flow and transport equations. The soil profile was discretized into 1-cm elements. An atmospheric boundary condition (Šimůnek et al., 2005) was implemented at the soil surface, which required specifying on a daily basis the irrigation rate, evaporation rate, and solution concentration in the irrigation water. The lower boundary was specified as a free drainage condition (Šimůnek et al., 2005).

Model Parameter Distributions

The effects of parameter uncertainty on predicted solute transport were investigated with Monte Carlo techniques. Probability distributions for the soil hydraulic parameters in Eq. [2–3] were determined using the Rosetta pedotransfer function model (Schaap et al., 2001). Rosetta contains a hierarchy of neural network-based models which require different levels of input data. We evaluated two models, the Rosetta textural class model, which estimates retention parameters and K_s based on a soil's textural class, and the SSCBD model, which estimates the same parameters based on the soil bulk density and the percentages of sand, silt, and clay. Rosetta also computes values for K_0 and L based on the estimated retention parameters. The Rosetta

Table 1. Soil physical characteristics and simulation model parameters.†

Soil material	Sand	Silt	Clay	Bulk density	θ_r	θ_s	$\log_{10}\alpha$	$\log_{10}n$	$\log_{10}K_s$	$\log_{10}K_0$	L
	%			g cm^{-3}	cm^3 cm^{-3}		$\log_{10}$ cm		$\log_{10}$ cm d^{-1}		
Clay loam	42	25	33	1.25	0.0857 (0.0099)	0.4811 (0.0095)	−1.8207 (0.0822)	0.1504 (0.0183)	1.4120 (0.2143)	0.6828 (0.2560)	−0.6640 (0.9691)
Silty clay	16	41	43	1.25	0.0980 (0.0084)	0.5070 (0.0120)	−1.8751 (0.0798)	0.1440 (0.0161)	1.3458 (0.1382)	0.5560 (0.2755)	−0.6768 (1.1238)
Sandy loam	78	11	11	1.6	0.0482 (0.0044)	0.3656 (0.0057)	−1.4545 (0.0461)	0.2016 (0.0149)	1.7423 (0.0748)	1.3020 (0.2511)	−1.0413 (0.7437)

† Estimated mean parameter values and, in parentheses, standard deviations.

parameter estimates also include parameter standard deviations. Table 1 gives parameters values and standard deviations estimated using the Rosetta SSCBD model with data for the soil materials used in the Skaggs et al. (2012) experiment. Table 1 gives estimates for both $K^* = K_s$ and $K^* = K_0$. The parameters θ_r, θ_s, and L were taken to be normally distributed, whereas K_s, K_0, n, and α were lognormally distributed (Schaap et al., 2001). Due to a lack of information about parameter correlations, the hydraulic parameters were considered uncorrelated in the Monte Carlo realizations.

The other uncertain model parameter expected to significantly affect solute transport simulations is the dispersivity, λ. Jury et al. (1991) note that typical reported values for λ are 0.5 to 2 cm in packed laboratory columns and 5 to 20 cm in field soils. Literature review articles indicate that λ is affected by soil texture, scale (soil volume and transport distance), boundary conditions (method of solute application and irrigation), and other experimental factors (Beven et al., 1993; Vanderborght and Vereecken, 2007; Bromly et al., 2007; Koestel et al., 2012). Various analyses of transport data sets in relation to the scale of observation has led to an informal rule-of-thumb that λ is often found to be equal to about 1/10 of the transport distance (Skaggs and Leij, 2002).

In principle it might be possible to prescribe or reduce uncertainty in λ by finding literature studies with comparable experimental parameters, but data compiled by Vanderborght and Vereecken (2007) indicate that unsaturated clayey systems, such as considered in the present work, are perhaps the least studied conditions for solute transport. Lacking information that would dictate an alternative, we specified λ to have a uniform distribution while considering different possibilities for the lower and upper bounds, as discussed below in the Results section.

Generalized Sensitivity Analysis

Generalized parameter sensitivity coefficients for the Monte Carlo simulations were determined by performing linear regression analyses of computed concentrations against model parameters. For N model parameters, let p_{ij} be the value of the jth parameter generated in the ith realization, and let C_i be the concentration computed for that realization at $t = T$ and $z = Z$. The basic model for the regression analysis is (Saltelli et al., 2005)

$$\tilde{C}_i = \tilde{p}_{i1}\beta_1 + \tilde{p}_{ij}\beta_j + \ldots + \tilde{p}_{iN}\beta_N + \varepsilon_i \qquad i = 1, \ldots, M \qquad [5]$$

where $\tilde{C}_i = (C_i - \mu_{C_i})/\sigma_{C_i}$ and $\tilde{p}_{ij} = (p_{ij} - \mu_{p_{ij}})/\sigma_{p_{ij}}$ are standardized variables; μ_{C_i}, $\mu_{p_{ij}}$, σ_{C_i}, and $\sigma_{p_{ij}}$ are the means and standard deviations of C_i and p_{ij}, respectively; β_j are standardized regression coefficients; ε_i is the error term; and M is the number of Monte Carlo realizations. A goodness-of-fit measure for the linear regression is given by the coefficient of determination,

$$R^2 = \frac{\sum(\tilde{C}_i^* - \mu_{\tilde{C}_i})^2}{\sum(\tilde{C}_i - \mu_{\tilde{C}_i})^2} \qquad [6]$$

where $\tilde{C}_i^*$ is the concentration predicted by the regression model, $\mu_{\tilde{C}i}$ is the mean of $\tilde{C}_i^*$, and $R^2 \in [0, 1]$. Although the model used in our work is not actually linear in its parameters, Saltelli et al. (2005) indicate that an R^2 value greater than about 0.7 is evidence that Eq. [5] is a reasonable approximation and that in such cases the regression parameters β_j can be interpreted as parameter sensitivity coefficients. The coefficients are global in the sense that their magnitude is affected by sensitivities over the whole parameter space, which is in contrast to classical sensitivity measures (e.g., Skaggs and Barry, 1996) that indicate sensitivity only at a single point in the parameter space (Saltelli et al., 2005).

Results and Discussion

Evaporimeter

Evaporimeter Water Flow

We first consider measured and predicted water flow and water potential in the evaporimeter. Although we are primarily interested in solute transport, we examine water flow here to verify that the general modeling approach is sound. The simulation model is driven by the surface boundary condition, which in this case was

specified based on daily irrigation and evaporation data that were available from direct gravimetric measurements (Fig. 2). Figure 3 shows measured and predicted soil water pressure heads at the 10- and 30-cm depths and measured and predicted drainage (outflow) rates (depth = 48 cm). The model prediction intervals shown in the figure are the 5th, 50th, and 95th percentiles of the model output distributions computed with the Monte Carlo method using M = 5000 parameter set realizations. Figures 3a–3c show results obtained using the Rosetta estimate for $K^* = K_0$, whereas Fig. 3d through 3f show results for $K^* = K_s$. The pressure head data in Fig. 3 were not used in any way in the model calculations. The drainage data were not used directly in the model calculations, but indirectly those data were used to determine the evaporation rate (Fig. 2) that was incorporated into the model surface boundary condition, and thus the results in Fig. 3c and 3f are not independent model predictions.

Figures 3a, 3b and 3d, 3e show that the soil water pressure head predicted with K_0 was in better agreement with measured data than was the pressure head predicted with K_s. With K_0 (Fig. 3a and 3b), greater than 90% of the daily pressure head readings fall within the bounds given by the 5th and 95th percentiles (shown as a shaded gray area). With K_s (Fig. 3d and 3e), the data generally fall outside the interval, with the predicted soil pressure head

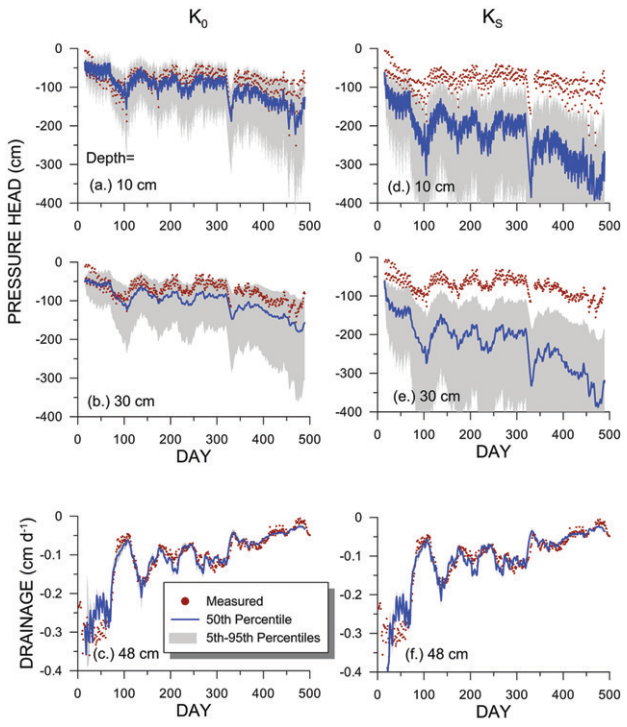

Fig. 3. Comparison of measured and modeled soil water potential and drainage in the evaporimeter. The gray shaded region indicates the interval between the 5th and 95th percentiles of the Monte Carlo output, whereas the blue line is the 50th percentile. Plots (a–c) show results obtained using the matching point conductivity $K^* = K_0$, whereas (d–f) show results obtained with the saturated conductivity $K^* = K_s$. In (d) and (e), a significant portion of the 5th–95th interval has been truncated at the lower limit of the y axis.

being lower than observed. The high-frequency oscillations in the measured and predicted pressure head at 10 cm are due to wetting/drying that occurred during/between irrigations. Model and data comparisons for pressure heads at the 15- and 45-cm depths were similar to those presented in Fig. 3 and are not shown.

Figures 3c and 3f show that whatever differences existed in the pressure heads modeled with K_0 and K_s, it made almost no difference with respect to the predicted drainage rates. The computed drainage rates for the two cases were nearly identical, with very little variability existing between Monte Carlo realizations, such that the interval between the 5th and 95th percentiles (again indicated with gray shading) is barely visible in Fig. 3c and 3f due to its narrowness. Although the data generally fall outside that prediction interval, the model calculation is, all things considered, a very good representation of the time course of the drainage rate. Overall, Fig. 3 indicates that the implemented modeling approach provides a good description of soil–water conditions in the evaporimeter, particularly with $K^* = K_0$.

Evaporimeter Solute Transport

Figure 4 shows comparisons of predicted and measured solute breakthrough in the evaporimeter drainage water (outflow). The hydraulic parameter distributions (and the water flow calculations) are the same as in Fig. 3. In Fig. 4a and 4d, the dispersivity λ was taken to be uniformly distributed between 2 and 10 cm. Absent any other information, these bounds would be a plausible estimate for making a modeling prediction, based on the following reasoning. The transport distance is 48 cm. The 10% rule-of-thumb discussed above suggests a dispersivity of about 5 cm; doubling that value gives our assumed upper bound of 10 cm. The assumed lower bound of 2 cm is near intersection of the upper limit of values reported for repacked soil column experiments and the lower limit reported in field studies, which seems appropriate considering that the evaporimeter is larger than a typical soil column and close to the size of a small field plot.

Overall, the model predictions in Fig. 4a and 4d follow the basic trend of the measured solute breakthrough curve, which includes some inflections not typically present in classical, Gaussian shaped curves. Recall that during the period when the evaporimeter irrigation water contained Br tracer, the irrigation water concentration (C_0) was constant. However, the evaporation and irrigation rates varied (Fig. 2), leading to a time-varying evapoconcentration of the applied water at the soil surface. Thus the surface experienced time-varying fluxes and concentrations, a more complex (and realistic) boundary condition than typically imposed in controlled solute transport experiments. The time-varying evapoconcentration rate produced the inflections in the measured and modeled breakthrough curves, and concentrations $C/C_0 > 1$.

The solute transport prediction made using K_0 (Fig. 4a) was better than that made using K_s (Fig. 4d). The 5th through 95th percentile prediction interval in Fig. 4a contains 75% of the data points versus

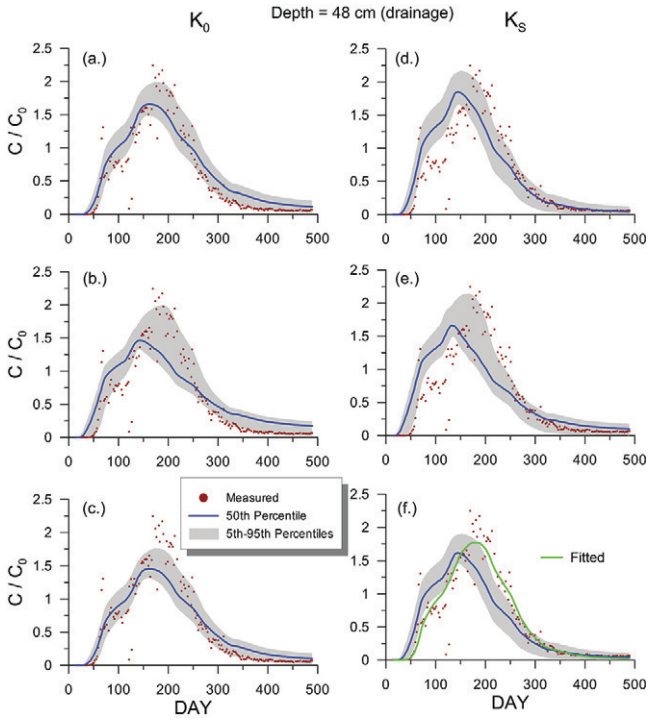

Fig. 4. Comparisons of measured and predicted Br concentration in the evaporimeter outlflow using various parameter sets. In plots a, c, d, and f, the dispersivity λ was uniformly distributed between 2 and 10 cm, and in Plots b and e, between 1 and 25 cm. In Plots c and f the input solute mass was scaled to match the output mass. See the text for a full description of the various parameter sets.

62% in Fig. 4d. However, evaluating the quality of the prediction interval in terms of the fraction of data points it contains is perhaps of limited value in this case. It is clear, for example, that the prediction with K_s shown in Fig. 4d is relatively inaccurate when the bulk of the solute is breaking through (say, Days 50–250) but is relatively accurate at later times on the tail end of the curve. Thus, the percentage of data points in the interval is in part dependent on the sampling scheme; more-or-fewer samples at early-or-late times would affect the percentage. Overall, the prediction of solute transport in terms of a prediction interval provides a more realistic representation of the concentration data than would a single breakthrough curve.

We next consider the effect of the assumed dispersivity distribution on the transport predictions. Figures 4b and 4e show results computed assuming significantly larger uncertainty, with λ assumed to be uniformly distributed between 1 and 25 cm. Compared with the previous results (Fig. 4a and 4d), the concentration distribution is broader and more asymmetric. However, the broader prediction interval encompassed about the same fraction of the data as before (72% in Fig. 4b and 66% in Fig. 4e), so in that sense the predictions for the alternative dispersivity distribution were not greatly different.

Because we are mainly interested in model predictions (rather than fitting), we specified the solute model boundary condition based on irrigation records, assuming nothing was known about the solute transport data. In solute transport experiments, it is common that solute mass balance is significantly different from 100%, and in evaluating process models, it is routine to scale or fit the model applied mass so that it agrees with the observed (Skaggs et al., 2002). In the evaporimeter experiment, the Br mass collected in the drainage water was about 88% the applied mass. To determine the effect of the mass balance error on the prediction accuracy, we repeated the calculations after adjusting the model irrigation water concentration so that the simulated applied solute mass agreed with the measured drainage mass. The results, shown in Fig. 4c and 4f, indicate that the predictions were not greatly different, with the prediction intervals encompassing 79% and 63% of the measured data points, respectively.

Generalized parameter sensitivity coefficients, $\beta_j(t)$, for the simulations of Fig. 4a are presented in Fig. 5a, and the corresponding $R^2(t)$ for the standardized regression model is given in Fig. 5b. Sensitivity results for the other simulations were similar and are not shown. The relatively high R^2 values in Fig. 5b indicate that the coefficients β_j of the linear model can be utilized for sensitivity analysis. Thus Fig. 5a shows that the model parameters having the greatest impact on the modeled outflow concentration and uncertainty were λ, K^*, and n. The least sensitive were θ_r and α. The relative sensitivities for model parameters are expected to be dependent on experimental conditions—an experiment with a surface boundary condition that imposed cycles of significant wetting and drying, for example, would likely have different sensitivities than the current experiment, where the soil was maintained at a high, unsaturated water content. Note that in Fig. 5 the low β_j and R^2 values at early times are because the sensitivity calculations are for the outflow concentration; at early times, solute has not reached the exit, and thus no sensitivity to the parameter values exists. Figure 4f shows the "optimal" simulated breakthrough curve resulting from a simultaneous optimization of the two most sensitive parameters, λ and K^*, based on a least-squares fit of the model to the solute breakthrough data. The optimized value for the conductivity, $K^* = 6.5$ cm d^{-1}, was close to the Rosetta mean estimate for K_0 (4.8 cm d^{-1}), and far out on the tail of the estimated distribution for K_s (Pr[$K_s < 6.5$ cm d^{-1}] = 0.003). The fitted dispersivity, $\lambda = 2.6$ cm, was near the low end of our assumed uniform parameter distribution.

We also considered model calculations using the Rosseta class average hydraulic parameters. However, the large uncertainty (standard deviation) in the parameter estimates complicates their use in simulations. The distributions for some of the parameters are sufficiently broad to encompass, with non-negligible probability, parameters or parameter combinations that are undefined (non-physical) or lead to numerical instabilities (e.g., $n \leq 1$, $\theta_r < 0$, $\theta_s < \theta_r$). While the possibility exists for developing rules for eliminating unusable parameter sets, we decided not to further pursue this approach at this time.

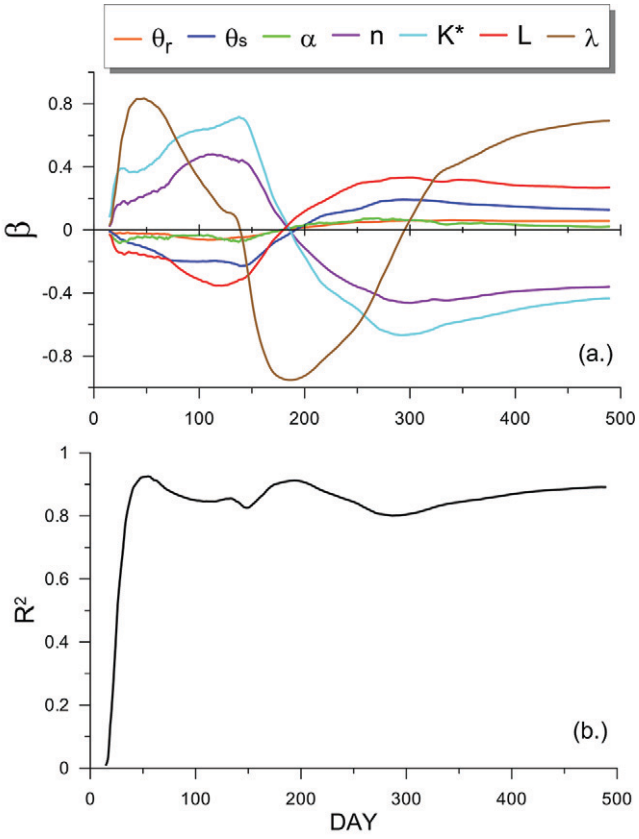

Fig. 5. (a) Generalized sensitivity coefficients, $\beta_j(t)$, for the model parameters, computed with respect to the outflow concentration, $C(t)$, shown in Fig. 4a. (b) The corresponding coefficient of determination, R^2, for the standardized regression model used in the sensitivity analysis.

Lysimeters

Lysimeter Water Flow

A difficulty arose in modeling the lysimeters due to the water balance. The net applied water in the lysimeters was expected to be the same as that measured in the (identically irrigated and situated) evaporimeter. Given that assumption, the measured lysimeter drainage was only about half of what was expected. Part of the discrepancy might be due a misestimation of the change in lysimeter water storage, and part might be due to the lysimeter evaporation differing somewhat from the evaporimeter evaporation. However, it is unlikely that these factors would be sufficient to account for the discrepancy. It appears that the main cause for the discrepancy was that, over the course of the 4 year experiment, frequent operation of the solution samplers removed a nonnegligible volume of water. The volume extracted cannot be determined directly because the sampling protocol, wherein the vacuum was left running for extended periods, produced an overflowing of small collection vials that was uncontrolled and unrecorded (the need for lengthy vacuum applications was due to the low conductivity of the soils). Indirectly, we can estimate the water loss based on the difference between the net applied water (assumed known from evaporimeter measurements) and the measured drainage.

Because of the water balance problem, simulations were done two ways. First, predictions were made without any consideration of the water balance discrepancy. Hence the simulations were a pure prediction based only on data recorded for the surface boundary condition. In a second set of simulations, we added a sink term to Eq. [1] to account for the water and solute extractions. The sink removed water and solute at a steady rate from the eight depths where the solution samplers were installed, such that the final simulated cumulative drainage was approximately equal to the average measured amount.

In the lysimeter simulations, the effects of K_0 vs. K_s were similar to those noted in the evaporimeter, so we present hereafter only the K_0 results in an effort to avoid overcomplicating the figures. Figure 6 shows comparisons of the measured and modeled drainage rate and pressure heads at three depths (30, 120, and 165 cm), one from each soil layer. Results for other depths were similar and are not shown. To improve legibility, only a subset of the very large number of measured tensiometer and drainage data points are shown. Data for the two experimental treatments (high or low EC irrigation water during Br application) are indicated with color: red symbols correspond to the low EC treatment (Lysimeters 1–6) and green symbols to the high EC treatment (Lysimeters 7–12). Monte Carlo results for simulations with the drainage correction are shown as a blue line (50th percentile) and gray interval (5th–95th percentiles). The red line is the 50th percentile for the uncorrected simulations. The size and shape of 5th to 95th interval about the 50th percentile in the uncorrected simulations was comparable to that in the corrected simulations and is not shown due to legibility considerations.

Figures 6a through 6c show that the predicted or modeled pressure head is generally lower than the measured values. The predictions made without drainage correction are in marginally better agreement with the data, with many of the data lying within or near the upper limit of the 5th–95th prediction interval (not shown), whereas in the simulations with drainage correction, the data are almost entirely outside the prediction interval. In Fig. 6d, the drainage rate predicted with the uncorrected simulations is clearly a poor fit to the data. The drainage rate obtained after correcting for the water balance is better, although the modeled drainage does not track the data as well as it did in the evaporimeter calculations. The range of variability among the measured lysimeter drainage rates is generally greater than the relatively narrow width of 5th to 95th prediction interval, whereas the opposite is true of the pressure head data, where the width of the prediction interval generally exceeds the variation among lysimeters. Note that the variability in water flow that existed among the lysimeters does not appear to correlate with the two experimental treatments (Skaggs et al., 2012).

Lysimeter Solute Transport

Figure 7 compares the measured Br data with the Monte Carlo results. Results for five profile depths and the drainage are presented. Results for the other depths were comparable and are

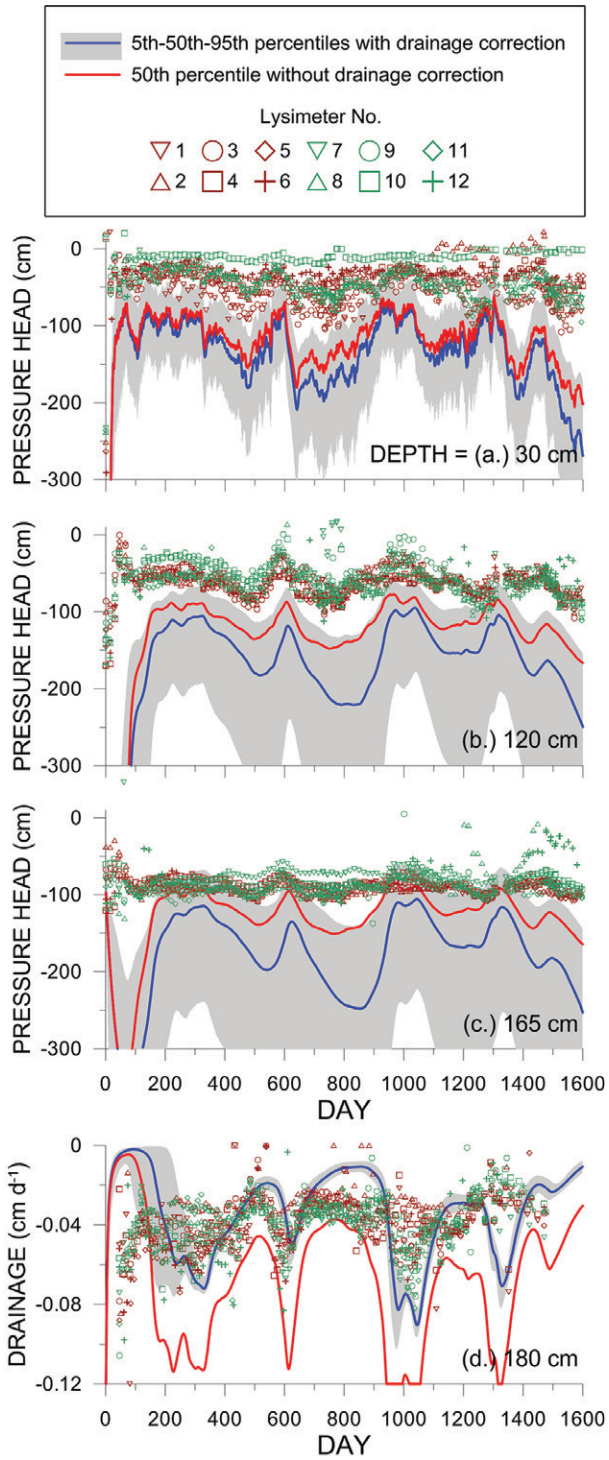

Fig. 6. Comparison of measured and modeled soil water potential and drainage for the lysimeters.

not shown. Only a subset of the data points measured for each breakthrough curve are shown (every third point is shown for solution samplers, every 10th point for drainage). In the Monte Carlo computations, the dispersivity was specified to be uniformly distributed between 2 and 20 cm.

Overall, the general time course of the simulations agrees with the data, except at later times in the high EC treatment lysimeters (green symbols), which will be discussed below. The simulations with and without drainage correction are nearly identical to one another at the shallowest depths (Fig. 7a and 7b). Deeper in the soil (Fig. 7c–7f), differences emerge, with the breakthrough computed with drainage correction increasingly lagging behind that computed without. The breakthrough computed with the corrected drainage appears to be in better overall agreement with the measured data, although in both cases the predicted concentrations generally exceed the measured data.

As can be seen from the red (low EC) and green (high EC) data points in Fig. 7, the two experimental treatments reported by Skaggs et al. (2012) produced distinctly different transport behaviors. For most of the salinization phase, Br concentrations increased identically in all lysimeters, with no apparent differences between treatments. But after about 1.5 yr, the breakthrough data from the two treatments diverged. The initial break occurred near Day 550 to 575, a time during the salinization phase in which the surface boundary was experiencing a diminishing evapoconcentration rate, such that the effective inlet concentration was decreasing, leading to a decrease in salt concentrations at shallow depths (note the irrigation water concentration was not changing). This period of relative leaching led to multi-peaked breakthrough curves near the surface (at deeper depths, those features were largely damped out). After the start of the actual irrigation leaching phase (Day 804), the bifurcation of the two treatments became more pronounced. The Br concentrations decreased readily in the low EC treatment lysimeters (1–6), whereas in the high EC lysimeters (7–12) an initial rapid decrease in Br was followed by a lengthy period of tailing (Skaggs et al., 2012). The reason for the different leaching behaviors is not known, although Skaggs et al. (2012) speculated that a type of salt sieving mechanism may have contributed.

Clearly the model tracks the low EC data better than the high EC data. To our knowledge, no model exists that could have predicted the differences in leaching behavior exhibited by the two irrigation treatments. Modeling of transport processes in clayey soils poses significant challenges due to the strong effect that the surface charge of clay particles has on soil hydraulic properties and on the mobility of solutes (Nielsen et al., 1986). Yet clayey soils with low infiltration rates are among those most likely to be impacted by salinity.

In terms of modeling uncertainty, the discrepancy between the model and the high EC data constitutes a "structural" model error that, in this case, is much more significant than the parameter uncertainty. From the standpoint of making a pure model prediction, it would not have been possible to anticipate this error. Clearly in this case the model would have underestimated the time or water needed to lower the salinity in the profile.

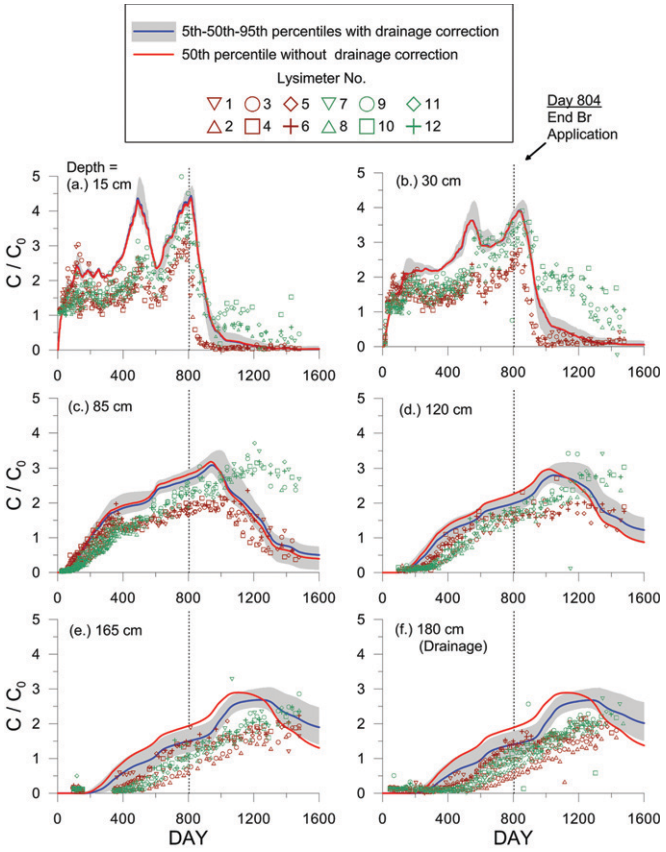

Fig. 7. Comparisons of measured and modeled Br concentrations for various depths in the lysimeters.

Aside from the structural errors, the width of the prediction intervals are fairly narrow relative to the range of transport variability that existed across replicated lysimeters, particularly at shallow depths. At deeper depths, the prediction interval is a reasonably good representation of the variability in the low EC lysimeters.

Figure 8 shows sensitivity coefficients computed for the hydraulic and transport parameters of the three soil layers. Sensitivities for the 21 parameters were evaluated with respect to the solution concentration at three depths, one in each layer. The R^2 results were similar to that given in Fig. 5 and are not shown. Figure 8a through 8c indicate that the soil concentration at 30 cm is, as expected, most sensitive to the parameters of the surface layer, and mostly insensitive to the parameters of the second and third layers. Similar to the evaporimeter results, the surface layer parameters with the largest sensitivity coefficients are λ, K_0, and n. Figure 8d through 8f show that at 120 cm (in the second layer), the concentration is again greatly impacted by the surface layer parameters, especially λ. Sensitivity to the second layer parameters is comparatively minor, a result affected by the relative thinness of the second layer (Fig. 1). The third layer parameters K_0 and L also impact the concentration in the second layer (Fig. 8f). At 165 cm, the surface layer dispersivity remains important (Fig. 8a), as do the parameters K_0 and L for the coarser third layer. The sensitivity results, in addition to being dependent on the boundary condition, are affected by the relative thickness of the three layers.

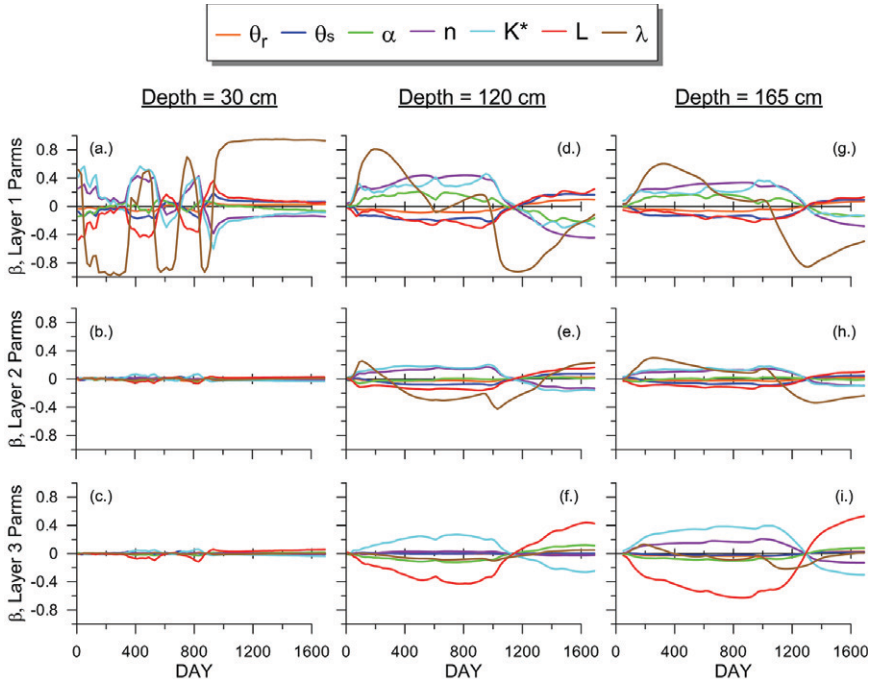

Fig. 8. Generalized sensitivity coefficients of the model parameters for the three soil layers, computed with respect to the solute concentration at the three indicated soil profile depths.

Conclusions

Monte Carlo techniques were used to propagate uncertainty in soil hydraulic and solute transport parameters. Simulations of solute transport were compared with Br transport measured in large lysimeters packed with clayey soil materials. The following conclusions may be drawn.

1. For the investigated unsaturated systems, simulations performed using the Rosetta estimate for K_0 as the matching point conductivity K^* were in better agreement with experimental data than simulations performed using the estimate for K_s.

2. Although specific information about dispersivity uncertainty is frequently lacking, plausible parameter bounds may be estimated based on literature studies.

3. Texture class average pedotransfer function uncertainty estimates for model parameters were sufficiently broad to include parameter values or combinations of values that are undefined (non-physical) or lead to numerical instabilities (e.g., $n \leq 1, \theta_r < 0$, $\theta_s < \theta_r$). Further work is needed to develop rules for eliminating unusable parameter sets.

4. Generalized sensitivity coefficients computed with regression analyses were useful for identifying the most significant model parameters. In a single layer system, the model parameters having the greatest impact on the modeled outflow concentration and uncertainty were λ, K^*, and n. The least sensitive were θ_r and α. In a three layer system, model parameters (λ, K^*, and n) for the surface layer had the highest sensitivity coefficients, even with respect to computing concentrations in deeper depths. The parameters K^* and L in the coarser bottom layer also significantly affected the outflow concentration. Sensitivity results are expected to be dependent on the boundary conditions imposed in the experiment.

5. Prediction intervals based on the propagation of PTF parameter uncertainties are more realistic in their representation of solute transport processes than any single model run, but in this study the generated intervals tended to somewhat underestimate the variability that existed in the transport data. This was particularly true with respect to solute transport at shallow depths.

6. Clayey soils are among the most likely to suffer from salinity problems, and they pose significant challenges for modeling transport. In a 48 cm tall, homogeneous soil profile, model prediction intervals provided a reasonably good description of a single, relatively "noisy" breakthrough curve. In replicated 180 cm tall, layered soil profiles, model structural errors limited the accuracy of the prediction intervals under one irrigation water treatment, whereas under another treatment the predictions tracked the time course of the data reasonably well but tended to overestimate solute concentrations. The experimental data were obtained in repacked soils; solute dispersion in undisturbed soils may differ (Elrick and French, 1966; Koestel et al., 2012). Additional work aimed at operational field testing of model prediction uncertainty is needed if advanced water management models are to reach their full potential.

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