Using data assimilation to identify diffuse recharge mechanisms from chemical and physical data in the unsaturated zone

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[1] It is difficult to estimate groundwater recharge in semiarid environments, where precipitation and evapotranspiration nearly balance. In such environments, groundwater supplies are sensitive to small changes in the processes that control recharge. Numerical modeling provides the temporal resolution needed to analyze these processes but is highly sensitive to model errors. Natural chloride tracer measurements in the unsaturated zone provide more robust indicators of low recharge rates but yield estimates at coarse time scales that mask most control mechanisms. This study presents a new probabilistic approach for analyzing diffuse recharge in semiarid environments, with an application to study sites in the U.S. southern High Plains. The approach uses data assimilation to combine model predictions and chloride-based recharge estimates. It has the advantage of providing probability distributions rather than point values for uncertain soil and vegetation properties. These can then be used to quantify recharge uncertainty. Estimates of moisture flux time series indicate that percolation (or potential recharge) at the data sites is episodic and exhibits interannual variability. Most percolation occurs during intense rains when crop roots are not fully developed and there is ample antecedent soil moisture. El Niño events can contribute to interannual variability of recharge if they bring rainy winters that provide wet antecedent conditions for spring precipitation. Data assimilation methods that combine modeling and chloride observations provide the high temporal resolution information needed to identify mechanisms controlling diffuse recharge and offer a way to examine the effects of land use change and climatic variability on groundwater resources.


1. Introduction and Background

[2] Characterization of groundwater recharge is critical for sustainable management of water resources, control of subsurface contamination, and better understanding of hydrologic and ecological variability. It is well known that the primary controls on recharge are meteorology, soil properties, vegetation, and topography. These controls interact to create the distinctive conditions that result in recharge. Uncertainties about control mechanisms make it difficult to predict long-term effects of climate change, meteorological variability, and land use change on groundwater resources.

[3] De Vries and Simmers [2002] categorize recharge as “diffuse” (or “direct”) when it originates from precipitation that infiltrates vertically from the surface directly to the water table. By contrast, nondiffuse (“localized” or “focused”) recharge travels laterally at (or near) the land surface and then collects in streams or topographic depressions before it infiltrates. Both diffuse and localized recharge often travel via preferential pathways, such as through cracks or root tubules, rather than exclusively through the soil matrix. Preferential flow is especially difficult to characterize or predict.

[4] Although diffuse recharge may occur infrequently in arid and semiarid climates, it can still have significant impact on the overall groundwater budget. Kearns and Hendrickx [1998] point out that small amounts of diffuse recharge spread over a large area can yield significant volumetric contributions to groundwater in semiarid regions of New Mexico. Also, in areas where deep-rooted vegetation has been replaced by shallow-rooted crops or pasture, diffuse recharge rates can increase significantly [e.g., Cook et al., 1989; Scanlon et al., 2007]. In fact, increases in diffuse recharge induced by land use change have created major environmental problems in Australia, where salt trapped in the unsaturated zone has been flushed into valuable ground and surface water reservoirs [Cook et al., 1989; Leanev et al., 2003].

[5] In this paper we examine the interacting processes that control diffuse recharge, in order both to better understand the relevant mechanisms and to provide a better basis for predicting impacts of land use and climate change on subsurface water supplies. Gee and Hillel [1988] observed
that diffuse recharge in semiarid regions is likely to occur episodically rather than continuously. This has been documented in a number of settings [see, e.g., Zhang et al., 1999a, 1999b; Lewis and Walker, 2002]. An understanding of the origin and timing of discrete events is needed for proper characterization of diffuse recharge. In particular, we need to be able to determine the relative importance of downward moisture movement driven by precipitation events and upward moisture movement driven by evaporation and root uptake. If downward forces prevail for even a brief period, infiltrating precipitation can move from the surface past the root zone and eventually become recharge. Otherwise, it is taken up by vegetation and/or evaporated, and there is little or no moisture left to recharge groundwater.

[5] Scanlon et al. [2002] provide a comprehensive review of common methods for estimating recharge. One option is to use numerical models of the unsaturated zone to predict recharge from precipitation observations and various soil and vegetation properties [e.g., Zhang et al., 1999b; Small, 2005; Keese et al., 2005]. Although numerical models are undoubtedly useful, many studies [e.g., Gee and Hillel, 1988; Allison et al., 1994; Phillips, 1994] caution against their application in semiarid environments. Because diffuse recharge rates in such settings can be quite small relative to precipitation and evaporation, they are very sensitive to uncertain model parameterizations and input errors. For this reason, tracer-based recharge estimation methods are favored by Gee and Hillel [1988] and Allison et al. [1994] in semiarid environments. Natural tracers such as meteoric chloride are particularly popular due to their ubiquitous availability and increased sensitivity at lower recharge rates.

[7] Chloride concentrations in the unsaturated and/or saturated zone are most often employed for recharge estimation using a simple chloride mass balance (CMB) approach, which assumes that, over the long-term, the average rate of chloride deposition with precipitation balances the rate of chloride flushed out of unsaturated zone soil water (below the root zone) [Scanlon et al., 2002]. When surface runoff/run-on is negligible (such as in low-relief areas), soil water chloride is of meteoric origin, and chloride is fully displaced via piston flow, this can be expressed as

\[ P[Cl_P] = R[Cl_{SW}], \]

where \( P \) is the precipitation rate, \( [Cl_P] \) is the atmospheric chloride concentration (accounting for wet and dry fallout), \( R \) is the percolation rate below the root zone, and \( [Cl_{SW}] \) is the soil water chloride concentration. Negligible amounts of chloride are generally taken up by plants, making the above an acceptable approximation. Although this steady state mass balance approach can provide robust average recharge estimates, it cannot resolve the fine time-scale dynamics that link diffuse episodic recharge to transient surface conditions (weather and changes in vegetation).

[5] Quasi-transient and generalized versions of chloride mass balance (CMB) provide some temporal information by associating particular portions of the unsaturated profile with particular times in the past [Cook et al., 1992; Murphy et al., 1996; Ginn and Murphy, 1997]. The chloride front displacement method tracks solute flushing caused by changes in land use [Allison and Hughes, 1983; Walker et al., 1991]. However, Cook et al. [1992] showed that dispersion and mixing greatly limit the temporal resolution of these alternatives. Chloride data do not appear to adequately capture seasonal effects, annual dynamics, or other short-duration events responsible for episodic recharge.

[5] In summary, it seems fair to say that numerical modeling provides temporally detailed, yet potentially inaccurate, recharge estimates, while chloride-based recharge estimation methods produce robust, but less detailed, time-integrated estimates when the CMB conditions cited above are met. Although the two methods are complementary, few studies have combined them to obtain recharge estimates that have the temporal detail and accuracy needed to fully describe episodic events. Some investigators [e.g., Cook et al., 1992; Flint et al., 2002; Scanlon et al., 2003] use chloride measurements to validate numerical models, but they do not actually combine the two sources of information.

[10] In this paper we estimate recharge with a probabilistic data assimilation approach that integrates model predictions and unsaturated zone data while properly accounting for sources of uncertainty. Data assimilation methods, including Kalman filtering and variational least squares methods, have been used in a number of other hydrological applications [e.g., Kitandis and Bras, 1980; McLaughlin et al., 1993; Reichle et al., 2001; Margulis et al., 2002; Reichle et al., 2002; Vrugt et al., 2005; Dunne and Entekhabi, 2006]. Here we use a particular data assimilation approach commonly known as importance sampling (discussed more fully in section 2). This approach generates populations of physically plausible model parameters (e.g., soil and vegetation properties), soil moisture profiles, and recharge histories that are consistent with model predictions and field observations. Importance sampling explicitly accounts for both model and measurement uncertainty by weighting each source of information according to its reliability.

[11] In the discussion that follows, we distinguish percolation, the moisture flux below the root zone (1.5 m in our study), and recharge, the moisture flux at the water table. The two are generally equivalent over the long term because percolation, which we presume is beyond the influence of evapotranspiration, eventually reaches the water table to become recharge (with some delay). Recharge is the quantity of most interest from the perspective of groundwater supply. However, its temporal dynamics are significantly attenuated, especially if the water table is deep. Because percolation responds more to episodic precipitation events and other surface conditions, it provides a clearer picture of the physical mechanisms that control recharge. For this reason, our analysis is based on estimates of percolation rather than recharge. However, our ultimate interest is in the effect of land use practices and climate on recharge.

[12] This paper demonstrates how importance sampling can be used to estimate episodic percolation in a semiarid region affected by land use change and to provide the insight needed to understand recharge mechanisms. Our estimates of percolation and related quantities are derived from physical and chemical field data collected at research sites in the semiarid southern High Plains (SHP) region of Texas. Over the past century, replacement of native grassland at these sites with rain-fed (dryland) cotton crops has
led to increased flushing of unsaturated zone chloride, resulting in increased diffuse recharge [Scanlon et al., 2007]. This land use change has provided a strong chloride signal that facilitates estimation of generally unobservable soil and vegetation properties.

Although CMB has been used in many past studies, Gee et al. [2005] suggest that chloride-based recharge estimates can be misleading when low chloride concentrations (due to increased flux) approach instrument detection levels. Those errors can be further compounded when soil water chloride is not fully flushed with piston flow. Good agreement between CMB and chloride front displacement calculations in the SHP indicate that these are not major concerns and that measured chloride concentrations are informative about flux rates at our study sites [Scanlon et al., 2007].

Our study of diffuse recharge mechanisms and related soil and vegetation properties begins in section 2 with a brief review of Bayesian data assimilation concepts. Section 3 illustrates the application of importance sampling to the diffuse recharge problem. Section 3 includes discussions of the field sites, the unsaturated zone model, selection of model inputs, and representation of uncertainty. Section 4 examines the percolation and property estimates obtained by assimilating data from the SHP field sites. These estimates indicate how episodic percolation is controlled by a combination of meteorological, soil, and vegetation factors. A comparison of percolation estimates with precipitation records and cropping schedule reveals the special conditions that make episodic percolation, and thus recharge, possible at agricultural sites such as the two sites considered here. These conditions are summarized in section 5.

2. Data Assimilation and Importance Sampling

The two main components of a data assimilation problem are a numerical model and a set of measurements. We assume these are described by a state equation model \( f \) and a measurement model \( h \), respectively:

\[
x_{1:T} = f(x_{0:T}, p, b_{1:T}, \varepsilon_{1:T})
\]

\[
y_{1:T} = h(x_{1:T}, \eta_{1:T}).
\]

where \( x_{1:T} \) is the vector of system states (predictive variables) defined over a time period of length \( T, x_{0} \) is the initial state vector, \( p \) is the parameter vector, \( b_{1:T} \) is the boundary condition vector over time, \( \varepsilon_{1:T} \) is the state model error vector not included in other inputs, \( y_{1:T} \) is the observation vector, and \( \eta_{1:T} \) is the observation error vector.

For the recharge problem of interest here, \( f \) represents a combined soil moisture and solute transport model; \( x \) includes soil moisture, chloride concentrations, and moisture fluxes at different depths; \( p \) includes soil and vegetation parameters; \( b \) includes meteorological and solute deposition forcing at the ground surface; and \( y \) includes soil moisture and chloride concentration measurements in a vertical unsaturated zone profile. Percolation (the moisture flux at 1.5 m) is a model output (diagnostic variable) that is determined completely by the model inputs and states. In our study, measurements at each site are taken at only one time, and thus (3) simplifies to

\[
y_{T} = h(x_{T}, \eta_{T}).
\]

Many model calibration methods are designed to estimate a single parameter set that provides a “best fit” to observations. When models and observations are highly uncertain, it may be more useful to provide probabilistic estimates that reveal the range of possible values rather than a single “best estimate.” In this case, the objective of the estimation procedure is to derive the conditional (posterior) probability density \( p(X|y) \) of an uncertain model input, state, or output (indicated by the generic symbol \( X \)). This conditional density conveys everything we know about \( X \) given uncertain information from the model and measurements.

Bayes’ theorem relates the conditional density \( p(X|y) \) to the unconditional (prior) probability density \( p(X) \) and to the likelihood function \( p(y|X) \), expressed as a function of \( X \) for a given measurement \( y \):

\[
p(X|y) = \frac{p(y|X)p(X)}{p(y)}.
\]

It is sometimes possible to derive closed form expressions for the unconditional probability densities of the model states and outputs by combining the state equation given in (1) with specified input probability densities. Such a closed form derivation is not possible for our recharge problem. Instead, we adopt a Monte Carlo approach and work with samples from the relevant densities rather than the densities themselves. Our approach to Bayesian data assimilation is carried out in three steps:

1. Generate equally likely unconditional realizations of uncertain model inputs (e.g., meteorological, soil, and vegetation properties) from specified input probability density functions.

2. Use Monte Carlo simulation to derive a corresponding set of equally likely realizations of the unconditional model states (e.g., the soil moisture and chloride concentration profiles) and model outputs (e.g., percolation). Each Monte Carlo sample includes a set of associated inputs, states, and outputs.

3. Use importance sampling to reweight each Monte Carlo sample to reflect its ability to match observations. The reweighted samples provide the information needed to construct approximate conditional probability densities for the model inputs, states, and outputs.

Monte Carlo simulation and importance sampling represent the probability densities appearing in (5) discretely, using a set of \( i = 1, \ldots, N \) sample vectors (\( X^{i} \)) containing input, state, and output variables, together with a set of associated unconditioned weights (\( w_{i}^{u} \)) or conditioned weights (\( w_{i}^{c} \)):

\[
p(X) \approx \sum_{i=1}^{N} w_{i}^{u} \delta(X - X^{i})
\]

\[
p(X|y) \approx \sum_{i=1}^{N} w_{i}^{c} \delta(X - X^{i})
\]

\[
\sum_{i=1}^{N} w_{i}^{c} = 1, \quad \sum_{i=1}^{N} w_{i}^{u} = 1.
\]
Figure 1. Importance sampling example with unconditional probability distribution (black curve), observation (dashed line), and conditional probability distribution (gray curve). The set of points $X'$ is drawn at random from the unconditional distribution and is indicated by the asterisks. Unconditioned and conditioned particle weights are represented by black and gray circle sizes, respectively. The points have equal unconditioned weights, but the conditioned weights are different, with higher values assigned to points closer to the observation. The weighted average of the $X'$ values is the mean of the conditional probability distribution shown.

where $\delta(\cdot)$ is the Dirac delta function. The model input variables of $X'$ are drawn at random from a population of equally likely prior samples that conform to a specified unconditional density $p(X)$ (step 1 above). The corresponding model state or output component of $X'$ is derived by running the simulation model with the particular set of random inputs (step 2 above). Usually only some of the inputs are treated as random variables, while the others are assumed to be deterministic (i.e., uncertainty is not accounted for). Because each sample generated in the Monte Carlo procedure is equally likely, the unconditional sample weights are all $w_U = 1/N$.

[22] The measurement conditioning process (step 3 above) is accomplished by adjusting the equal weights associated with the Monte Carlo samples to reflect the effect of measurements. In particular, the weights $w_C$ of the conditional density are given by substituting (6), (7), (8), and $w_U = 1/N$ into (5) to obtain

$$w_C = \frac{p(y|x')}{\sum_{i=1}^{N} p(y|x_i')}. \tag{9}$$

For example, if measurement errors are additive, then $y_T = h(x_T, \eta_T) = h(x_T) + \eta_T$, and the likelihood function appearing in (9) may be computed from

$$p(y|x') = p_{y|x'}(y|x') = p_{y|x'}[y - h(x_T')], \tag{10}$$

where the subscripts on the probability densities refer to the random variables of interest while the arguments refer to the threshold values used to evaluate probabilities. The measurement error probability density $p_{y|x'}[\eta_T]$ is usually presumed to have a convenient closed form, such as a Gaussian or uniform density. This density should reflect the effects of instrumentation and recording errors, as well as representativeness errors that account for scale differences between the observation support and model grid cells.

[23] The importance sampling approach to Bayesian conditioning outlined above ensures that more weight is given to samples that provide a good match to observations. In our application, this has the effect of shifting the probability densities of observed states toward the measurements. This is illustrated with a simple univariate example in Figure 1.

[24] Importance sampling methods are commonly encountered in particle filters, which are sequential Bayesian data assimilation algorithms. Particle filters are popular in tracking and signal processing [Djurić et al., 2003], and they have also been applied to hydrologic problems [Moradkhani et al., 2005; Zhou et al., 2006; Pan et al., 2008; Weerts and El Serafy, 2006; Smith et al., 2008]. Our importance sampling procedure is a nonsequential (single time) adaptation of the sequential importance resampling (SIR) particle filter [Arulampalam et al., 2002].

[25] Note that importance sampling can be inefficient if the unconditional probability density of the states is a poor estimate of the conditional density. In this case, many samples will be needed to obtain a few low-probability realizations that match the data. This problem is exacerbated when the state vector is high-dimensional, and generation of samples is computationally demanding [Daum and Huang, 2003]. Because our recharge problem considers only a single vertical profile and has a relatively small number of uncertain states and inputs, importance sampling is computationally feasible, especially if care is taken to specify physically reasonable unconditional probability densities. Importance sampling has the distinct advantage of deriving conditional samples directly from Bayes’ theorem without relying on the implicit Gaussian and linearity assumptions required in Kalman filtering and least squares variational methods, or on heuristic measures used in calibration approaches [McLaughlin, 2007].

3. Application of Importance Sampling to the Recharge Problem

[26] The basic objective of our Bayesian data assimilation procedure is to estimate the conditional probability densities of percolation at various times and the conditional densities of the uncertain model inputs used to predict percolation. The desired conditional densities are constructed from a large number of sample values and weights using the Monte Carlo simulation and importance sampling procedures described in section 2. In our case, each Monte Carlo sample includes values for uncertain model inputs (e.g., vegetation and soil properties and meteorological variables), values for the model states (e.g., soil moisture and chloride), and values for model outputs derived from the inputs and states (e.g., moisture fluxes used to quantify percolation). The weights obtained from the importance sampling procedure indicate the relative probability of each sample. The basic components of the data assimilation process are shown in Figure 2 and described in sections 3.1–3.4.
3.1. Measurements at the Study Sites

[27] The measurements used in our data assimilation study were obtained from study sites located in the southern High Plains (SHP) region of the United States. This 75,000-km² region spans parts of northern Texas and eastern New Mexico and is characterized by flat topography and about 16,000 draining playas or ephemeral lakes (see Figure 3). The SHP is considered to have a semiarid climate with a mean annual precipitation in the range of 375–500 mm. About 75% of precipitation falls during May through October in convective storms. In parts of the SHP with native grassland and shrubland, recharge occurs almost exclusively through playas [Wood and Sanford, 1995; Scanlon and Goldsmith, 1997].

[28] Replacement of natural vegetation with shallow-rooted crops (much of it rain-fed cotton) in the early 1900s led to increases in diffuse recharge. The natural vegetation was mostly replaced with cotton, often grown without irrigation in continuous monoculture. Over 2003 to 2006, Scanlon et al. [2007] drilled and sampled 20 unsaturated zone boreholes in rain-fed cotton areas of the SHP (indicated in Figure 3) to investigate the effect of the land use change on recharge. Scanlon et al. [2007] found widespread occurrence of flushed meteoric chloride in their profiles. This result is similar to Australian studies that found low chloride concentrations in the unsaturated zone following clearing of eucalyptus trees [Cook et al., 1989; Kennet-Smith et al., 1994].

[29] This evidence of flushing and downward moisture movement following land use change is in marked contrast to the slightly upward moisture fluxes generally observed in natural interplaya environments. The CMB method described by equation (1) should be applicable for the relatively flat study area. Simulations further support this with insignificant runoff amounts. CMB calculated fluxes in the SHP ranged from 4.8 to 70 mm/a in individual profiles under cropland [Scanlon et al., 2007]. Such changes in recharge above the natural level near zero have led to rises in water table levels, which could, in turn, eventually lead to waterlogging and possibly compromise water quality through salinization [Scanlon et al., 2005].

Figure 2. Diagram of recharge estimation approach. Random samples of states and outputs are generated via multiple model runs using different inputs, as represented by multiple arrows in the diagram. Conditional statistics of the uncertain variables are obtained by associating the conditioned weights obtained from importance sampling with the sample values.

Figure 3. Southern High Plains (SHP) map (adapted from Scanlon et al. [2007, Figure 1]). Inset shows location of SHP in Texas and New Mexico. Data sites used in this study are fully flushed D06–02 and partly flushed L05–01.
Half of the chloride profiles examined by Scanlon et al. [2007] exhibited low chloride concentrations throughout, suggesting that they were fully flushed with postdevelopment moisture fluxes. The remaining profiles exhibited high concentration bulges at depth, suggesting the presence of a postdevelopment region affected by downward recharge lying above a predevelopment dry region that experienced little or no recharge. The positions of chloride bulges in the partially flushed profiles convey important information about the flux history, because deeper profile locations reveal conditions further back in time. Scanlon et al. [2007] used this profile information to derive chloride front displacement estimates that corroborated CMB results. In the analysis presented here, we examine a representative profile from each group: the fully flushed profile D06–02, and the partially flushed profile L05–01. Soil samples for these profiles were collected on 14 February 2006 and 26 May 2005, respectively.

Unsaturated zone profile measurements given by Scanlon et al. [2007] include chloride concentration, soil moisture, matric potential, and soil texture (percent clay, silt, and sand). Chloride concentrations were obtained by first drying soil samples, adding water, and shaking, and then using ion chromatography to measure concentrations in the supernatant. Soil moisture was measured gravimetrically. Data from the National Atmospheric Deposition Program (http://nadp.sws.uiuc.edu/) provided the basis for the atmospheric chloride deposition rates from precipitation, which were doubled to account for dry deposition and correspond to prebomb 36Cl/Cl ratios found in the region [Scanlon and Goldsmith, 1997]. Further details on measurement methods are provided by Scanlon et al. [2007].

In this study, we assimilate soil moisture and chloride concentration data and use soil texture data to identify unconditional soil property densities. Chloride and soil moisture measurements in the root zone were omitted because the numerical unsaturated zone flow and transport model used in this study does not accurately simulate the transient conditions in this region [Cook et al., 1992; Tyler and Walker, 1994]. Matric potential measurements from the SHP sites were not used because they appear to include inconsistencies with soil moisture and chloride observations in some partially flushed profiles [Scanlon et al., 2007]. Chloride and soil moisture measurements below the root zone provided sufficient constraint on model parameters and moisture fluxes. In summary, our assimilation study relies on soil moisture and chloride profile measurements and model predictions from several depths below the root zone, representing snapshots in time at each site (14 February 2006 for D06–02 and 26 May 2005 for L05–01). These measurements are plotted in Figure 4, and related information reported by Scanlon et al. [2007] is summarized in Table 1.

### Table 1. Site Data From Scanlon et al. [2007]

<table>
<thead>
<tr>
<th></th>
<th>D06–02</th>
<th>L05–01</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude, longitude</td>
<td>32.63°N, 102.09°W</td>
<td>33.93°N, 102.61°W</td>
</tr>
<tr>
<td>Water table depth</td>
<td>10 m</td>
<td>36 m</td>
</tr>
<tr>
<td>[Cl−] in precipitation</td>
<td>0.34 mg/L</td>
<td>0.28 mg/L</td>
</tr>
<tr>
<td>Elapsed time since land use change (time used in this work)</td>
<td>67–75 years (71 years)</td>
<td>70–85 years (76 years)</td>
</tr>
<tr>
<td>Chloride mass balance (CMB) recharge estimate from Scanlon et al. [2007]</td>
<td>70 mm/a</td>
<td>14 mm/a</td>
</tr>
</tbody>
</table>
moisture is simulated in SWAP using a finite difference solution of the well-known Richards’ equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - T_a(t,z). \quad (11)$$

Solute transport is simulated using a finite difference solution of the advection-dispersion equation for nonsorbing solutes, assuming no uptake by roots:

$$\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial z} \left[ \theta(D_{diff} + D_{disp}) \frac{\partial C}{\partial z} - qC \right]. \quad (12)$$

In these equations, $\theta$ is volumetric soil moisture, $h$ is matric potential, $K$ is unsaturated conductivity, $T_a$ is water uptake by roots, $C$ is solute concentration in the pore water, $D_{diff}$ and $D_{disp}$ are molecular diffusion and dispersion coefficients, and $q$ is moisture flux. The molecular diffusion coefficient is set to 1 cm$^2$/d for the solute diffusion coefficient in free water, which is within the range of values listed for chloride by Robinson and Stokes [1965]; the dispersion coefficient is derived from a dispersivity of 2 cm [Cook et al., 1992].

Surface boundary conditions for (11) and (12) and the sink term (transpiration) in (11) are determined from daily meteorological inputs and vegetation parameters. The simple (nondynamic) crop option of SWAP was implemented, for which vegetation parameters over the growing season are user-specified. Soil evaporation is capped at potential evaporation ($E_p$), which is calculated from the Penman-Monteith equation [Monteith, 1981] assuming no crop resistance and a decay factor based on crop foliage. An empirical evaporation option in SWAP based on that of Black et al. [1969] was selected to calculate actual evaporation ($E_a$) over a time step using

$$E_a = \min(E_p, E_{Darcy}, E_{emp}). \quad (13)$$

$E_{Darcy}$ is calculated from the average hydraulic conductivity ($K_{1/2}$) between the top node at $z_1$ and the surface, and the gradient between the top node soil water pressure ($h_1$) and soil water pressure that is in equilibrium with air humidity ($h_{atm}$):

$$E_{Darcy} = K_{1/2} \left( \frac{h_{atm} - h_1 - z_1}{z_1} \right). \quad (14)$$

$E_{emp}$ over a time step $dt$, at time $t_{dry}$, since a significant rain event, is

$$E_{emp}(t_{dry}) = \beta \left( t_{dry}^{1/2} - (t_{dry} - dt)^{1/2} \right), \quad (15)$$

where $\beta$ is an empirical parameter that describes evaporative properties for the surface soil layer. Potential evapotranspiration (PET) is found using the Penman-Monteith equation, including crop resistance. Potential transpiration is then computed from PET less $E_p$. Actual transpiration in SWAP depends on root density and solute and water stresses as well as on potential transpiration. Since we assume no significant interaction between the groundwater and the observed profiles, we set a free gravity drainage bottom boundary condition below the measured depths (i.e., the bottom matric potential gradient is set to zero).

In our data assimilation procedure, the vector $X$ of values to be estimated includes SWAP model states (soil moisture, chloride concentrations, and moisture fluxes over the entire simulation period) and model inputs. The simulations began at the time of land use change (1935 for D06–02 and 1930 for L05–01) and ended at the measurement date (February 2006 for D06–02 and May 2005 for L05–01).

3.3. Model Inputs and Uncertainty

In our approach to data assimilation, unconditional probability densities of the model states are approximated with a Monte Carlo approach that derives individual samples of the states from samples of uncertain model inputs. Because the conditional state and parameter values derived in importance sampling are just reweighted versions of the unconditional sample values, it is especially important to ensure that the unconditioned model inputs include values that can reproduce observations to within measurement error. The importance sampling procedure identifies these values and gives them increased weight when it constructs the conditional population. In our study, we found that a sample population of about 30,000 was sufficient to yield an adequate number of high weight samples.

Although nearly any model input has some uncertainty, this does not imply that all inputs must be varied in a Monte Carlo analysis. Since assumptions must be made about the nature of randomness included in such an analysis, it is best to focus on uncertain variables that are known to have an important effect on predictions so that the number of probabilistic assumptions can be kept to a minimum. We assume here that uncertainty in the model is conveyed solely through parameter and boundary conditions, thus eliminating the residual model error term $\epsilon$ in equation (2). The uncertain model inputs include vegetation and soil parameters and meteorological inputs. Whenever possible, nominal input values and probabilistic assumptions are based on data reported in the literature. Some decisions are made according to preliminary sensitivity tests. The following paragraphs summarize the probabilistic assumptions made for each type of uncertain model input. The model’s initial solute and matric potential values at the time of land conversion (~70 years before measurements) are deterministic and reflect conditions currently found under native grassland areas. Simulations showed little sensitivity to the exact profiles used for the dry and saline initial conditions.

3.3.1. Vegetation Parameters

Because our simulations begin at the time of land use change, vegetation parameters are only needed for cotton. Because of the lack of detailed crop schedule data, we assumed that crop emergence began every year on 15 May and that harvest occurred on 19 October [Keese et al., 2005]. For most vegetation parameters, time-varying nominal values over the growing season were chosen based on the literature, and these were multiplied by an independent time-invariant uniformly distributed random variable with mean 1.0. Multiplicative uncertainty was held constant over time to avoid averaging out perturbation effects over the growing season.
The vegetation parameters used in our study are summarized in Table 2. Sensitivity tests indicated that root depth has the greatest impact on percolation. Consequently, this parameter was assigned a reasonably high level of uncertainty. Although the cited sources often report maximum rooting depths greater than the nominal 1 m used here [e.g., Bland and Dugas, 1989; Sarwar and Feddes, 2000], smaller values were specified to reflect the fact that most moisture uptake is in the shallower active root zone. The root density profile was assigned a deterministic set of values based on those of G. L. Ritchie et al. (see http://pubs.caes.uga.edu/caespubs/pubs/PDF/B1252.pdf), with greatest root density near the surface. In effect, the large uncertainty in rooting depth accounts indirectly for uncertainties in the depth profile. Water and solute stress parameters were also assigned deterministic values from Sarwar and Feddes [2000] and the SWAT manual [Kroes and van Dam, 2003], because they have minimal impact on percolation in our simulations.

### Table 2. Vegetation Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nominal Value</th>
<th>Literature Basis</th>
<th>Unconditional Uncertainty</th>
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<tbody>
<tr>
<td>Root depth</td>
<td>1 m (max)</td>
<td>Bland and Dugas [1989], Sarwar and Feddes [2000], Droogers [2000], Bland and Dugas [1989]</td>
<td>time-constant multiplicative uniform noise [0.5, 1.5]</td>
</tr>
<tr>
<td>Leaf area index (LAI)</td>
<td>5 (max)</td>
<td>Askew and Wilcut [2002]</td>
<td>time-constant multiplicative uniform noise [0.75, 1.25]</td>
</tr>
<tr>
<td>Crop height</td>
<td>0.9 m (max)</td>
<td>Kroes and van Dam [2003]</td>
<td>multiplicative uniform noise [2/3, 4/3]</td>
</tr>
<tr>
<td>Minimal crop resistance</td>
<td>90 s m⁻¹</td>
<td>Sarwar and Feddes [2000]</td>
<td>none</td>
</tr>
</tbody>
</table>

The root density profile of each soil was assigned a deterministic set of values based on those of G. L. Ritchie et al. (see http://pubs.caes.uga.edu/caespubs/pubs/PDF/B1252.pdf), with greatest root density near the surface. In effect, the large uncertainty in rooting depth accounts indirectly for uncertainties in the depth profile. Water and solute stress parameters were also assigned deterministic values from Sarwar and Feddes [2000] and the SWAT manual [Kroes and van Dam, 2003], because they have minimal impact on percolation in our simulations.

#### 3.3.2. Soil Parameters

Soil texture data in the study region provided the basis for the soil parameters used in the simulations. SWAT uses the van Genuchten-Mualem soil moisture retention and unsaturated hydraulic conductivity functions given by van Genuchten [1980]. The six soil parameter needed for these functions were determined from soil texture using the pedotransfer model Rosetta [Schaap et al., 2001]. Because Keese et al. [2005] found soil layers to significantly affect recharge, we used heterogeneous parameters that vary between layers centered at the soil texture measurement locations for each study site. The uncertainty for the vertically heterogeneous soil parameters was attributed to two sources: (1) the texture values entered into Rosetta and (2) the pedotransfer functions imbedded in Rosetta. Because nearby soils can be expected to be similar, percent clay and silt profile densities in the SHP were assumed to be stationary Gaussian first-order autoregressive (AR-1) random processes over depth. Length-scale (\(\alpha_{\text{AR1}}\)) and standard deviation (\(\sigma_{\text{AR1}}\)) parameters were based on texture data collected from 24 boreholes in the SHP [Scanlon et al., 2007]: \(\alpha_{\text{AR1}} = 0.9964\) and \(\sigma_{\text{AR1}} = 1.7\) for percent clay, and \(\alpha_{\text{AR1}} = 0.9956\) and \(\sigma_{\text{AR1}} = 1.9\) for percent silt, using a 1-cm depth resolution.

The percent clay and silt profile samples used for our data assimilation study were conditioned on the point texture observations obtained from D06–02 and L05–01 (shown in Figure 4), assuming additive Gaussian measurement errors with standard deviations of 5% clay and silt. The conditional random sample profile was averaged over each soil layer interval to give a single layer value. The resulting layer values for percent clay, silt, and sand were entered into Rosetta, which provided corresponding layer values for the van Genuchten-Mualem soil parameters. Possible errors in the Rosetta pedotransfer function were represented by AR-1 depth-correlated perturbations added to the parameter values produced by Rosetta. Perturbations are scaled according to parameter uncertainty values produced by Rosetta.

#### 3.3.3. Meteorological Inputs

Meteorological inputs needed for SWAT are the chloride concentration in precipitation, daily precipitation, minimum and maximum air temperature \((T_{\text{min}}\) and \(T_{\text{max}}\), solar radiation, vapor pressure, and wind speed. The chloride concentrations in precipitation were obtained from Scanlon et al. [2007] (see Table 1). The four meteorological stations with long-term historical daily data closest to our study sites are in Amarillo, Lubbock, Lamesa, and Midland, Texas (see Figure 3). Information on the daily meteorological data available at these four stations is provided in Table 3. Daily (or even finer) precipitation data are needed to resolve the episodic precipitation events that largely control diffuse recharge in semiarid areas.

The closest station to D06–02 is Lamesa, which is 15 km away. The closest station to L05–01 is Lubbock, which is a relatively distant 77 km away. Data for each study site were taken from the closest station when possible. Missing data at the closest station were reconstructed from precipitation and temperature records at the other stations, or by sampling seasonally appropriate historical records for the station with missing data. Further details on the reconstruction of daily meteorological series for each study site are provided by Ng [2008]. Preliminary simulations showed that recharge response is relatively insensitive to nonprecipitation meteorological values. As a result, only precipitation was represented as uncertain.

Uncertainty was included in the daily rainfall intensity to account for (1) differences between rainfall at the study sites and the meteorological stations, and (2) observation errors at the meteorological station. Uncertainty in
the timing of individual precipitation events was not included because it did not significantly influence percolation characteristics over the approximately 70 years study period, from which recharge mechanisms were inferred. Instead, uncertainty is included only in the daily rainfall intensities on days that are recorded as rainy at the meteorological stations.

[48] A simple random rainfall intensity model was constructed to produce different temporal daily rainfall intensity means and standard deviations for the different samples generated in the data assimilation procedure. The resulting rain series from the model have the same pattern of rain occurrence as that recorded at the meteorological stations, but the daily rain intensities on rainy days are randomized to account for uncertainty. While such a model cannot generate the true rainfall series at the observation sites, it makes it possible to include in the analysis uncertainty in temporal rainfall statistics. Details are given by Ng [2008].

[49] The chloride mass flux rate, which is the product of [Cl] and the precipitation P, is uncertain. Since available data are insufficient to warrant an explicit distinction between chloride concentration and precipitation uncertainties, we account for the net effect of these uncertainties on the chloride mass flux through the precipitation term alone.

3.4. Measurement Error

[50] The measurement error probability density plays a key role in importance sampling because it determines, through the likelihood function, the conditional weight \( w_C \) assigned to each Monte Carlo sample. For this reason, care should be taken to properly account for the factors that contribute to measurement error. In our study, gravimetric soil moisture measurements (g/cm\(^2\)) were assumed to have additive zero-mean Gaussian observation errors \( \omega_{yg} \) that are independent at different depths. The associated volumetric soil moisture values used for data assimilation can be written

\[ y_g = \rho_g y_s = \theta + \rho_g \omega_{yg}, \]  

where the bulk density \( \rho_g \) is set to 1.6 g/cm\(^2\), the value used for the results reported by Scanlon et al. [2007]. We selected a standard deviation of \( \sigma_{\omega_{yg}} = 0.03 \) for \( \omega_{yg} \). This value is intended to account for errors introduced during the soil collection, weighing, and oven-drying process. Note that treating bulk density as an uncertain parameter would result in volumetric soil moisture and chloride concentration data values that differ from those reported by Scanlon et al. [2007]. To maintain consistency with that work, we assume that bulk density is deterministic and constant. All uncertainty related to soil moisture measurements is represented through the gravimetric soil moisture observation error. We selected a standard deviation of \( \sigma_{\omega_{yg}} = 0.03 \) for \( \omega_{yg} \). This value is intended to account for errors introduced during the soil collection, weighing, and oven-drying process.

[51] As described in section 3.1, measurements of chloride concentration in the pore water \( y_C \) were derived from the measurement of chloride concentration in the sample supernatant \( y_S \), using the following relationship:

\[ y_C = \frac{R_{EYS}}{y_S} = \frac{R_{EYS}}{\theta_g + \omega_{yg}}, \]  

where the extraction ratio \( R_E \) is the mass of water added to the dried sample per mass of dried soil. For the same reason as bulk density, exact \( R_E \) values used for the results by Scanlon et al. [2007] were implemented as deterministic values. As a controlled experimental input, actual \( R_E \) should have little uncertainty. Additive and multiplicative Gaussian chloride measurement errors were used to account for the ±0.1 mg/L instrument error for ion chromatography [Scanlon, 2000] and the 9% mean difference between split tests for the chloride data [Scanlon et al., 2007], respectively. This gives the following expression for the supernatant concentration measurement:

\[ y_S = S + \omega_{S1} + S \omega_{S2}, \]  

where \( S = C \theta_g/R_E \) is the true supernatant concentration and \( \omega_{S1} \) and \( \omega_{S2} \) are independent with means of 0 and 1, respectively, and standard deviations of \( \sigma_{S1} = 0.1 \) mg/L and \( \sigma_{S2} = 0.1 \).

[52] Evaluating \( p(y_S|y_C,C,\theta) \) is problematic because (17) is nonlinear in \( \omega_{yg} \), making \( y_C \) non-Gaussian. We deal with this problem by expanding (17) about \( \omega_{yg} = 0 \), substituting (18) for \( y_S \), and ignoring higher order terms. This gives

\[ y_C = C + C \varepsilon_1 + \varepsilon_2 \]  

where \( \varepsilon_1 = \omega_{S2} - \sqrt{\omega_{S2}^2 \omega_{yg}} / \theta_g \) (20) and

\[ \varepsilon_2 = \frac{R_E \omega_{S1} \omega_{yg}}{\theta_g} - \frac{R_E \omega_{S1} \omega_{yg}}{\theta_g^2}. \]  

Table 3. Micrometeorological Data Availability and Sources for 1930–2005 in the U.S. Southern High Plains

<table>
<thead>
<tr>
<th>Station (MAP(^a))</th>
<th>Precipitation</th>
<th>Temperature</th>
<th>Solar Radiation/Vapor Pressure/WIND</th>
<th>Data Source(^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lamesa (470 mm)</td>
<td>1930–2005 (~750 missing)</td>
<td>1930–2005 (~850 missing)</td>
<td>none</td>
<td>NCDC</td>
</tr>
</tbody>
</table>

\(^a\)Mean annual precipitation for 1961–2005.

The conditional mean and covariance of the errors $\varepsilon_1$ and $\varepsilon_2$ are then

$$E[\varepsilon_1 | C, \theta] = E[\varepsilon_2 | C, \theta] = 0$$

(22)

$$\sigma^2_{\varepsilon_1} = E[\varepsilon'_1 | C, \theta] = E[\varepsilon_1 | C, \theta] = \sigma^2_{\varepsilon_2} + \frac{\rho^2_{\varepsilon_1 \varepsilon_2} \sigma^2_{\varepsilon_1}}{\theta^2}$$

(23)

$$\sigma^2_{\varepsilon_2} = E[\varepsilon'_2 | C, \theta] = E[\varepsilon_2 | C, \theta] = \sigma^2_{\varepsilon_2} + \frac{\rho^2_{\varepsilon_1 \varepsilon_2} \sigma^2_{\varepsilon_1}}{\theta^2}$$

(24)

$$E[\varepsilon'_1 | \varepsilon'_2 | C, \theta] = E[\varepsilon_1 | \varepsilon_2 | C, \theta] = 0$$

(25)

The primes represent the mean-removed variables. To facilitate our likelihood function calculations, we assumed that $\varepsilon_1$ and $\varepsilon_2$ were Gaussian with the means, variances, and covariance given in (22)–(25). Then, after determining the conditional covariance between soil moisture and chloride concentrations, the Gaussian likelihood function for a particular depth can be described with the following mean and covariance:

$$E\left[ \begin{bmatrix} y_c \\ y_0 \end{bmatrix} \mid C, \theta \right] = \begin{bmatrix} C \\ \theta \end{bmatrix}$$

(26)

$$\text{Cov}\left( \begin{bmatrix} y_c \\ y_0 \end{bmatrix} \mid C, \theta \right) = \begin{bmatrix} C^2 \sigma^2_{y_c} + \sigma^2_{y_0} - \frac{C \sigma^2_{y_c}}{\theta} \\ \frac{C \sigma^2_{y_c}}{\theta} - \sigma^2_{y_0} \sigma^2_{y_1} \end{bmatrix}.$$}

(27)

### 4. Results and Discussion

#### 4.1. Soil Profiles and Long-Term Recharge

The importance sampling procedure provides a set of weighted samples that may be used to estimate conditional probability densities, statistics, and other quantities that can shed light on the mechanisms that control episodic diffuse recharge. The importance sampling results obtained for our study sites are summarized in Figure 5 (top), which shows the conditional weights assigned to each of the simulated samples. These weights reflect the quality of fit between each sample and the soil moisture and chloride measurements, as determined by the likelihood function.

The black lines plotted in Figure 5 (bottom) show the chloride and soil moisture profiles for the 100 most highly weighted conditional samples ($w_c > 8 \times 10^{-4}$ for D06–02 and $w_c > 0.002$ for L05–01). The gray lines show a random sample of 100 equally weighted unconditional samples. It is apparent that the importance sampling procedure selects, out of the large sample of unconditional profiles, the relatively small number that gives the best fit to the observations. Each of these high weight samples corresponds to a particular model simulation based on a particular set of physically plausible inputs.

It is useful to compare percolation values from our Monte Carlo and importance sampling procedure with traditional chloride mass balance recharge values derived from the same data sets. For this purpose, we computed long-term average percolation for each Monte Carlo sample by dividing the cumulative percolation over the approximately 70 year simulation period by the simulation time (i.e., the time from land use change until the observation time at the study site). Over such time scales, long-term average percolation and recharge are essentially equivalent.

Figure 6 compares the long-term recharge probability densities obtained from the conditional (unequal) and unconditional (equal) weights. Negative values indicate downward fluxes. The unconditional densities have long tails, demonstrating high uncertainty. By contrast, the conditional densities are narrower, with peaks that are very close to the steady state CMB estimates. The conditional peak for the fully flushed D06–02 site is shifted noticeably toward greater downward flux values. The partially flushed L05–01 site has a conditional density that does not differ as dramatically from the unconditional density as D06–02, yet its uncertainty is substantially reduced. The significant shifts and uncertainty reductions in the conditional percolation densities demonstrate that chloride measurements can contribute significantly to unconditional Monte Carlo predictions derived solely from a numerical model.

#### 4.2. Model Parameters

Our data assimilation approach has the advantage of providing information on unobservable model inputs, such as soil and vegetation properties, as well as on model states and recharge values. Conditional parameter estimates can be used to make deterministic or probabilistic recharge predictions under different climate conditions or agricultural practices. These predictions are more robust than those derived from unconditional parameter estimates because they are constrained by available observations.

The strongest impact of observations on the conditional probability distributions were for maximum rooting depth, certain shallow soil parameters, and the evaporation parameter $\beta$. Beyond providing estimates of individual parameters, the weights assigned by importance sampling can be used to identify the groups of parameter values that are most consistent with observations. This makes it possible to describe the distinctive conditions needed to generate episodic diffuse recharge. The basic idea can be illustrated by considering the unconditional and conditional bivariate probability densities (Figure 7) for two particular model inputs: the maximum root depth and the evaporation parameter $\beta$. The diagonal strip of higher probability apparent in the conditional bivariate density plotted in Figure 7 indicates that deep roots are most likely to occur when the parameter is low. Equation (15) suggests that evaporation is greater when the evaporation parameter is large. A greater rooting depth yields more transpiration. The observed profiles are possible only if these two elements, which compete for moisture, are properly balanced. This balance is achieved by selecting parameter values in the high-probability region of Figure 7.

Data-conditioned relationships among other vegetation parameters and soil parameters over depth are given by Ng [2008]. Many weakly related unconditional parameters show notable conditional correlations. Such probabilistic assimilation results provide a way to identify key interactions among the soil, vegetation, and meteorological factors that control recharge.
4.3. Recharge Dynamics and Mechanisms

The major result of our data assimilation study is a set of high-resolution conditional percolation samples that are constrained by field observations. Such information is not available from either numerical modeling or traditional CMB alone. The fine temporal resolution provided by our approach is especially useful because it provides insight about the conditions that control episodic percolation. Significant uncertainty shown earlier in unconditioned parameters and long-term recharge indicate that percolation time series produced with unconditioned parameters can be

![Figure 5](image5.png)

Figure 5. (top) Conditioned (posterior) samples have unequal weights, unlike the equiprobable unconditioned samples. (bottom) Model samples with significant conditioned weights (black) are compatible with observations (symbols); unconditioned model results are in gray.

![Figure 6](image6.png)

Figure 6. Probability densities for unconditional (dashed) and conditional (solid) long-term recharge; chloride mass balance (CMB) estimate is indicated in gray. These and all subsequent probability densities shown were obtained from a kernel density estimator with a Gaussian kernel function.

![Figure 7](image7.png)

Figure 7. (top) Unconditional and (bottom) conditional bivariate distributions for evaporation parameter and root depth. The two parameters have independent and uniformly distributed before conditioning. Importance sampling reduces uncertainty, creating a region of higher probability in the space of possible parameter values.
misleading. Here we show that conditioning percolation time series on data even reveals some differences in temporal patterns between the two study sites, despite compatible meteorology and similar range of unconditional percolation simulations (Figure 5). This underscores the importance of data conditioning in identifying recharge dynamics and mechanisms.

4.3.1. Recharge Time Series

Conditional estimates of weekly precipitation and flux below the root zone are shown in Figures 8, 9, and 10, each of which focuses on a progressively narrower range of the simulation period. Figure 8 provides information on the frequency and magnitude of percolation events over the entire historical period, while Figures 9 and 10 show details that help reveal recharge mechanisms.

Figure 8 demonstrates that flux below the root zone in SHP has been highly episodic with large interannual variability over the ~70 year test period. Some years, such as 1941, with the annual highest precipitation, were dominated by very high recharge, while other periods, such as the early 1950s, which had a long-term drought, and the mid-1990s had virtually no recharge. At D06–02 there was very little recharge between major events. At L05–01 there was some upward flux at the reference 1.5 m depth. This suggests that the finer soil in L05–01 was more likely to retain moisture for roots in the top 1 m of the soil.

Interannual recharge variability at our study sites may be related, at least in part, to known climatic processes. Kurtzman and Scanlon [2007] found a statistically significant correlation between the summer Southern Oscillation Index (representing El Niño) and wet winters in the SHP ($P < 0.001$). Gurdak et al. [2007] analyzed historical rainfall records and groundwater levels in the High Plains for known climate cycles and identified signatures of both the Pacific Decadal Oscillation (10–25 years) and El Niño–Southern Oscillation (ENSO) (2–6 year) in their data. Our data assimilation procedure enables us to directly estimate and compare percolation in the SHP for known El Niño years.

coincident. A number of high-intensity percolation events directly followed El Niño episodes, such as in 1941 and 1992 for both D06–02 and L05–01 and in 1986 for D06–02. Although other El Niño years did not coincide with intense percolation events, some of the years did coincide with longer-duration, low-intensity events. These include 1973 and 2003 for D06–02 and 1958 and 1986 for L05–01. No large percolation events occurred in 1997–1998, even though this is generally considered to be the largest El Niño year of the twentieth century. We need to look at finer temporal resolution to understand how wet El Niño winters may or may not affect recharge in the SHP.

Figure 9 shows that percolation at our study sites varies greatly within the year. Although annual precipitation might provide a convenient and tempting indicator for recharge, strong percolation events are clearly not determined by rainfall on that time scale. For example, 1991 and 1992 had almost identical total precipitation amounts at D06–02, yet only 1992 experienced significant percolation. Comparable annual rainfall fell at L05–01 in 1961 and 1962, with only the former yielding significant percolation. It appears that high rainfall intensity is a better predictor of recharge than high annual rainfall. This is demonstrated during 1985 and 1992 at D06–02 and 1957 and 1967 at L05–01.

However, high weekly rain intensity alone is not sufficient to guarantee high-percolation events. Heavy rainfall events in 1991 at D06–02 and in 1965 and 1966 at L05–01 failed to produce much recharge. A close examination of Figure 9 reveals that high-intensity rainfall events were generally unable to trigger recharge during the middle to late part of the growing season. This applies to the three examples cited above. It appears that heavy rainfall cannot escape plant uptake during periods when the root system is mature. Thus episodic recharge is most likely to occur in response to intense rainfall outside the growing season.

This reasoning is supported by the observation that the relatively small precipitation events occurring during the winter generally yield some low, but discernible, percolation. This can be seen in 1984–1985, 1986–1987, and 1991–1992 for D06–02 and in 1957–1958 and 1960–1961 for L05–01. Some of the years coincide with wet El Niño winters. Although these small winter percolation events may not make a significant contribution to total recharge, they often precede larger percolation events that occur when more intense rainfall arrives at the start of the growing season. This probably occurs because small winter rainfall events increase antecedent soil moisture. This raises soil hydraulic conductivity which, in turn, causes more water to be transported through the root zone during subsequent early summer rains. Similar behavior has been observed in southeastern Australia, where fallow years appear to increase episodic recharge by boosting root zone moisture [Zhang et al., 1999b]. Such conditions explain the large percolation events at D06–02 during 1987 and 1992 shown in Figure 9, as well as the L05–01 percolation events.
in 1958 and 1961 following wet winters. In fact, the presence of winter rain preceding strong spring rains seems the key difference between 1991 and 1992 at D06–02 and 1961 and 1962 at L05–01. These years have similar annual precipitation histories, but much different recharge responses.

The above discussion indicates that antecedent moisture resulting from above-average winter rains, often seen during ENSO events, creates the conditions needed to obtain high recharge during intense spring rains. By contrast, dry conditions that prevail during the growing season, when crops take up most available moisture, make high-percolation events unlikely during the late summer and early fall, even when rainfall is intense. Late-year percolation events are rare at L05–01, where finer soils facilitate evapotranspiration of available moisture.

The spread of values shown in Figures 8–10 reveals the uncertainty in the percolation time series generated by our probabilistic approach. The flux histograms shown at selected time slices in Figure 9 show that there is a high certainty that both sites experienced negligible downward flux between isolated high-percolation events, with some probability of a slight upward flux at the end of the growing seasons at L05–01. This indication that downward moisture flux is very likely to be zero for extended periods between intense percolation events reinforces our characterization of percolation in the SHP as an episodic phenomenon. Figure 10 focuses on an even smaller time range, showing the evolution of a particular high-intensity recharge event over several weeks in the summer of 1987. At this resolution, uncertainty about the exact timing and magnitude of the percolation peak is significant. This is reflected in the percolation histograms shown in Figure 10 (bottom). However, all of the histograms and samples are consistent with the observation that a major event with percolation values over 10 mm per week occurred. This event followed a moderate rainstorm occurring at the end of an unusually wet spring and before maturation of the crop root system. The mechanisms generating this event and other events in the historical record are consistent with the discussion presented above.

### 4.3.2. Summary Statistics

Although diffuse recharge in semiarid regions is dominated by relatively short-term episodic events, monthly trends and other summary statistics are helpful for characterizing seasonal patterns. Figure 11 shows box plots that reveal monthly variations in the conditional probability densities of monthly average rainfall, rainfall intensity, and recharge at the two study sites over the approximately 70 year simulation period. These plots show that May–July generally contributed most of the recharge at both sites, even though the rainy season extends from May through October. This confirms observations from the sample time series in Figures 8–10, which indicate that little moisture escapes fully developed roots. Although both sites have similar seasonal flux patterns, only the coarser-textured D06–02 site experiences winter recharge. In fact, L05–01 on average experiences a small net upward (positive) flux during the months of September, October, and November. Less than 25% of the recharge at our SHP sites occurs during the three driest months of the year (December–February). By comparison, 20–50% of episodic recharge in Western Australia is believed to occur during the dry season [Lewis and Walker, 2002].

The ensemble spread shown in the box plots of Figure 11 also reveals that percolation uncertainty scales with precipitation rather than percolation magnitude. For example, late growing season percolation values exhibit greater spread than values during the less rainy winter months, even though the median percolation values are close to zero. Uncertainty in precipitation intensity appears to have a greater impact on percolation uncertainty during the summer when there are more rainy days. Precipitation uncertainty is further amplified by soil and vegetation parameter uncertainty in the root zone, which is most active during the rainy growing season.

The SHP monthly average percolation values tend to lag monthly average precipitation, reflecting the travel time through the root zone soil column to 1.5 m depth. This effect varies with season, as indicated by the correlation results plotted in Figure 12. Figure 12 confirms a time lag of a month or more during most times of the year. However, note the abrupt halt in correlation between rainfall and recharge starting in August, when the system memory is effectively reset. This reflects the fact that nearly all moisture from previous months has been extracted by roots. Figure 12 suggests that May–July recharge at L05–01 is controlled mostly by rainfall occurring after March, and...
May–July recharge at D06–02 may be affected by rainfall from as early as the previous November. Overall, May rainfall seems most important for determining May–July recharge, because it is the only high-rainfall month (in terms of total amount and intensity) without significant root density. Correlations between rainfall and recharge are generally stronger at D06–02, a result which suggests that soil at this site is more conductive and responsive.

The cumulative plots in Figure 13 show how much of the percolation at each site comes from high-intensity rainfall.

**Figure 11.** Box plots of conditional mean monthly precipitation, daily precipitation intensity, and percolation. Box lines indicate the first, second (median), and third quartiles; whiskers show data within another 1.5 times the interquartile range; and dots represent outliers. Spread shown is over ensemble of simulations, not over time. Most percolation occurs in late spring/early summer at the study sites.

**Figure 12.** Correlation between conditional monthly precipitation and percolation in same and later months. Abbreviated month labels start with September. Off-diagonal correlations indicate time lag between precipitation and resulting percolation. Note that correlations are negative because downward percolation is defined as negative.
episodic events. Figure 13 (top) shows the fraction of cumulative percolation over the historical period associated with events having a peak weekly percolation more negative than a given value. Figure 13 (bottom) shows the number of events having a peak weekly percolation more negative than a given value. We define a recharge event period as the time interval between successive inflection points (changes in the sign of the second derivative) in the weekly percolation time series. The recharge event magnitude is the peak weekly percolation value during the event period. We performed a cumulative percolation analysis for every sample in our conditional simulation distribution. Figure 13 plots the median of all percolation fractions or events counts as well as the first and third quartiles.

Figure 13 shows that 50% of the recharge at D06–02 comes from percolation events of about 9 mm per week strength or greater, which only occurred about 20–30 times over the entire 71 year period, or typically about once every 2.5 years. About 50% of the recharge at L05–01 originates from events of about 7 mm per week. These occurred even more rarely than at D06–02, only about once every 6 years. Recharge at L05–01 can be characterized as more episodic than at D06–02, considering that percolation events were about 40% less common than at D06–02. Furthermore, the single most extreme recharge event at L05–01 (in 1941) surpassed that of D06–02 in magnitude, and it contributed nearly 10% of the total L05–01 percolation over the 76 year historical period. It should be noted, however, that D06–02 had more occurrences of moderately intense percolation events (>20 mm per week peaks). Monthly tallies of percolation events confirm that most high-magnitude events occur in the spring, with occasional large events in the autumn at D06–02.

5. Summary and Conclusions

This paper presents a probabilistic recharge estimation approach that integrates numerical modeling, which is sensitive to errors in uncertain inputs, and unsaturated zone moisture and chloride measurements, which do not contain enough information to provide fine time-scale recharge estimates. By combining these two imperfect sources of information, we are able to identify the episodic events that account for most of the diffuse recharge at our semiarid southern High Plains study sites.

The Monte Carlo and importance sampling approach adopted here provides a probabilistic characterization of recharge and related model inputs and states. Probability densities are inferred from a large set of samples, each corresponding to a model simulation based on a particular set of randomly generated inputs. Unconditional (or prior) densities are computed by weighting all samples equally, without considering measurements. Conditional (or posterior) densities are weighted unequally, with the weight for each sample assigned according its ability to match soil moisture and chloride measurements.

Long-term recharge probability densities conditioned on observations from our study sites shifted significantly away from unconditional densities derived solely from the model toward the steady state value obtained from a traditional chloride mass balance (CMB) analysis. The conditional densities were also narrower than their unconditional counterparts, indicating less uncertainty. The long-term recharge values at the two study sites were about 40–65 mm/a for the site with coarser soil and about 10–15 mm/a for the site with finer soil.

Conditional model input probability densities from the two study sites indicate that soil moisture and chloride measurements provide the most information about surface soil properties and rooting depth. The marginal densities of most other model parameters did not change significantly after conditioning. Some of the conditioned parameters were highly correlated, indicating that unique parameter values cannot be identified solely from moisture and chloride measurements. However, the parameter correlation
patterns, as exemplified in the plot of bivariate conditional probability densities, identify the combinations of parameter values (e.g., root depth and evaporation parameters) required to explain observed recharge patterns. Overall, the conditioning process narrows the set of possible input combinations, giving a better picture of uncertain soil and vegetation properties at the study sites. This type of uncertainty reduction cannot be obtained in a deterministic model calibration that focuses only on point estimates of individual input variables.

[78] Our study uses percolation (moisture flux at 1.5 m depth, just below the root zone) to analyze recharge mechanisms. Our model-based data assimilation procedure provides conditional percolation probability densities at a fine time scale, enabling us to examine individual percolation events that generate recharge. Percolation at the two sites appears to be highly episodic and variable over the years and seasons, with 50% of long-term percolation originating from events occurring only once in about 2.5 years at the site with coarser soils, and once in about 6 years at the site with finer soils. In fact, at the finer-textured site, a single rare intense episodic event probably contributed almost 10% of the net percolation over the 76 year study period.

[79] Conditional probability densities for monthly percolation show that, on average, most recharge occurs in the early growing season (May–July), when rains are heavy yet roots have not reached full maturity. This time of year also has the highest-magnitude percolation events, which typically follow high-intensity rainfall. In contrast, heavy rains in the middle to late growing season rarely trigger appreciable recharge, especially at the finer-textured L05–01 site. Rain that does fall during the winter dry season tends to provide weak but sustained recharge. Furthermore, these winter events often provide the antecedent moisture conditions that facilitate strong recharge peaks in the late spring, when rains can be intense and crop roots are not yet well established. Thus wet winters, sometimes brought by El Niño events, can contribute to both total and high-intensity recharge by directly yielding weak winter recharge and providing moist soil conditions for springtime recharge. Overall, the recipe for high recharge at our study sites seems to be a combination of moderate winter rainfall, which provides antecedent moisture, followed by intense spring rainfall events that occur at times when root uptake is small.

[80] Data assimilation techniques that rely on both models and field observations provide the flexibility and temporal resolution needed to identify the factors responsible for episodic recharge. Probabilistic approaches such as the combination of Monte Carlo simulation and importance sampling used in our study are able to identify the combinations of meteorological conditions and soil and vegetation properties that facilitate recharge. Episodic percolation events that give rise to recharge may occur infrequently in semiarid regions, but they can account for a significant flux of water to subsurface aquifers. Improved understanding of such events, derived from models and field observations, should enable us to make better predictions of the impacts of land use and climate change on subsurface water supplies.

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